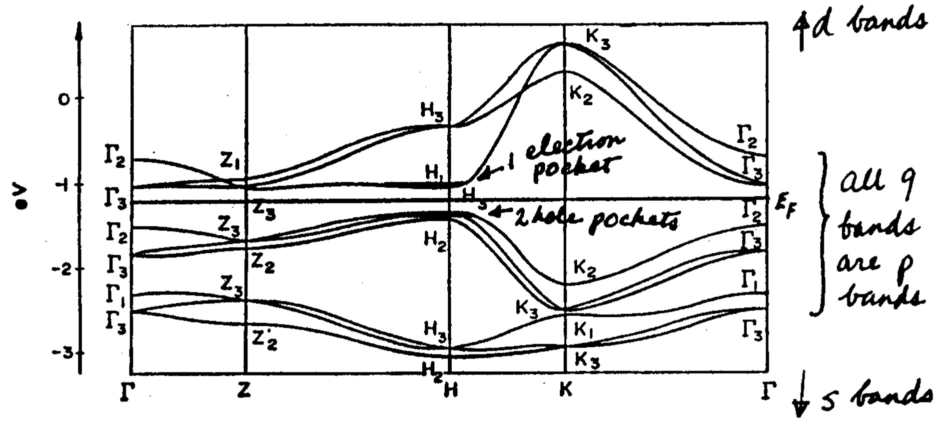
SOLUTIONS FOR PROBLEM SET #2

1)



(a) Since there are 3 Te atoms per unit cell and each atom has 4 valence p electrons. There are altogether 12 electrons per unit cell and they fill exactly 6 bands. Hence the Fermi level must lie in the band gap between the 6th and the 7th bands. See diagram.

(b) All the bands shown in the band diagram are p bands. They came from 3 Te atoms with each one contributing 3 p bands. Bands resulting from 5s and 5d atomic levels are below and above the band diagram, respectively.

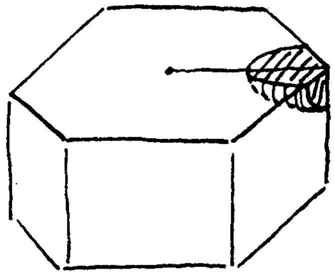
(c) Carrier pockets formed by thermal excitation will be at H point due to the narrowest band gap there. One 1/6 electron pocket and two (H_3 doubly degenerate) 1/6 hole pockets will be formed at H. (H is at zone boundary and therefore are not full pockets.) Howere, there are 12 equivalent H points inside the 1st B.Z. Hence there are

$$12 \times 1/6 = 2 \text{ full electron pockets}$$

$$12 \times 1/6 \times 2 = 4 \text{ full hole pockets}$$

(d) The shape for electron and hole pockets is a ellipsoid of revolution. Effective masses will be heavier along H-Z direction than along H-K direction from the curvatures of the bands around H.

$$\left(m^{*\,-1}_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j} \right)$$



(e) This depends on whether the light is heavily absorbed by exciting electrons from valence band(s) to unoccupied conduction band(s).

With $\lambda = 5000\,\text{Å}$,

$$E = \hbar\omega = \hbar 2\pi c/\lambda$$

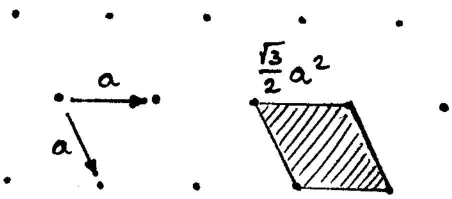
$$= \frac{0.658\times10^{-15}\ \text{eV-sec} \times 2\pi \times 3\times10^{8}\ \text{m/sec}}{5000\times10^{-10}\ \text{m}}$$

$$= 2.5\ \text{eV}$$

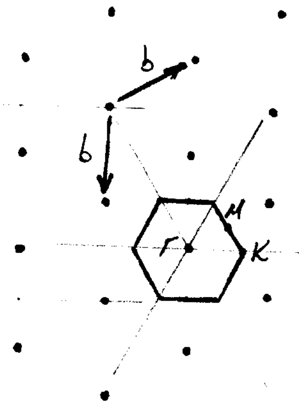
From the band diagram, this energy would excite electrons in the valence band from H to K to Γ. However the joint density of states there is small due to a huge difference in curvatures between the conduction bands and valence bands. Hence the absorption of light at $\lambda = 5000\,\text{Å}$ is small and the sample is transparent to visible light.

② Trigonal Lattice (a - lattice vector length)
2 electrons per atom.

$\bar{r}$ - space



$\mathbf{k}$ - space



$$a \cdot b \cdot \cos(30) = 2\pi$$

$$\Downarrow$$

$$b = \frac{4\pi}{\sqrt{3}a}$$

$$n = \frac{2}{(2\pi)^2}\int d^2k = \frac{2}{4\pi^2}\cdot \pi k_F^2 = \frac{2}{\text{unit cell}} = \frac{4}{\sqrt{3}a^2}$$

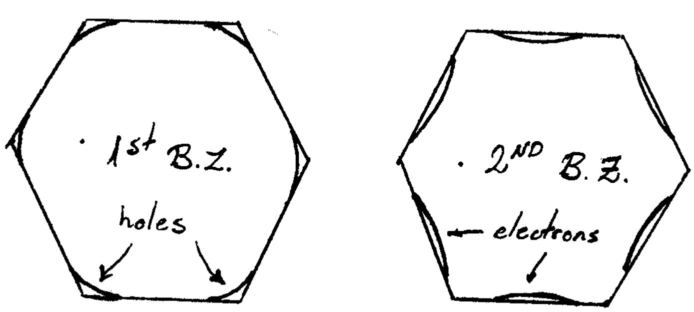
$$k_F = \left(\frac{8\pi}{\sqrt{3}a^2}\right)^{1/2} = \left(\frac{16\pi^2}{3a^2}\cdot\frac{\sqrt{3}}{2\pi}\right)^{1/2} = \left(\frac{\sqrt{3}}{2\pi}\right)^{1/2}\cdot b = 0.525\,b$$

$$|k|_{\Gamma\text{-}M} = \frac{1}{2}b = 0.5\,b$$

$$|k|_{\Gamma\text{-}K} = \frac{1}{3}\cdot 2b\cos 30 = \frac{2}{3}\cdot\frac{\sqrt{3}}{2}b = \frac{\sqrt{3}}{3}b = 0.577\,b$$

$$k_{\Gamma\text{-}M} < k_F < k_{\Gamma\text{-}K} \quad \text{(as expected!)}$$

$$A_{B.Z} = 6\cdot\frac{1}{2}\left(\frac{\sqrt{3}}{3}b\right)^2\cdot\frac{\sqrt{3}}{2} = \frac{\sqrt{3}}{2}b^2 = \pi k_F^2 \quad \text{(as expected!)}$$



3 electron pockets

2 hole pockets

$$A_{sector} = \frac{1}{2}k_F^2(\theta - \sin\theta)$$

$$= \frac{\sqrt{3}}{4\pi}b^2(0.62 - 0.58) = 0.0055\,b^2$$

$$= \frac{4\pi}{\sqrt{3}}\frac{1}{a^2}(0.62 - 0.58) = 0.29/a^2$$

$$\theta = 2\cos^{-1}\left(\frac{0.5b}{k_F}\right) = 35.5^\circ = 0.62\text{ rad}$$

$A_{\text{electron pocket}} = 0.011\,b^2$ (1.3% $A_{B.Z}$)

$A_{\text{hole pocket}} = 0.0165\,b^2$

3.

a) For intrinsic carriers only,

$$E_F^e = \frac{E_g}{2} - \frac{3}{4} k_B T \ln (m_h/m_e)$$

$$n_{intrinsic} = 2\left(\frac{\sqrt{m_c m_h}\, k_B T}{2\pi \hbar^2}\right)^{3/2} e^{-E_g/2k_BT} \qquad m_h^{3/2} = m_{heavy}^{3/2} + m_{light}^{3/2}$$

$$\sim 10^6/cm^3 \ll 10^{16}/cm^3 = N_{donor}$$

For the concentration of electrons thermally ionized into the conduction band

$$N_{d^+} = \frac{N_d}{1 + 2e^{(E_d - E_F)/k_BT}}$$

Now $E_d = 13.6\,eV \dfrac{m_e}{m_o} \dfrac{1}{\varepsilon^2} = 4.23\, meV$

$n_h \ll n_e$ and $N_d^+ \simeq n_e$

$$n_e = 2\left(\frac{m_c k_B T}{2\pi \hbar^2}\right)^{3/2} e^{-E_F/k_BT} \approx \frac{N_d}{1 + 2e^{(E_d - E_F)/k_BT}}$$

Making substitutions

$$\left(\frac{m_e k_B T}{2\pi \hbar^2}\right)^{3/2} = \left(\frac{1}{\lambda}\right)^3 \qquad \lambda = \text{thermal wavelength}$$

$$e^{-E_F/k_BT} = x \quad \Rightarrow \quad E_F(T) = -k_B T \ln x$$

We get $n_e = \frac{2}{\lambda^3} x \approx \frac{N_d}{1 + 2x\, e^{E_d/k_BT}}$

$$2x\left(1 + 2x\, e^{E_d/k_BT}\right) = N_d \lambda^3$$

$$4x^2 e^{E_d/k_BT} + 2x - N_d \lambda^3 = 0$$

$$x = \frac{-2 \pm \sqrt{4 + 16 N_d \lambda^3 e^{E_d/k_BT}}}{8 e^{E_d/k_BT}}$$

Take +ve sign

$$x = \frac{-1 + \sqrt{1 + 4 N_d \lambda^3 e^{E_d/k_BT}}}{4 e^{E_d/k_BT}}$$

$$E_F(T) = k_B T \ln\left(\frac{4\, e^{E_d/k_BT}}{\sqrt{1 + 4 N_d \lambda^3 e^{E_d/k_BT}} - 1}\right)$$

b) $E_F(300k)$ and $E_F(30K)$ substitute value of T into a

$E_F(300k) = 0.1\ eV$ below E_c

$E_F(30k) = 40 meV$ below E_c

c) Using $n_e = 2\left(\frac{m_e k_B T}{2\pi \hbar^2}\right)^{3/2} e^{-E_F/k_BT}$

$$n_e(300K) = \frac{2}{\lambda^3} e^{-E_F(300K)/k_BT} \approx 10^{16}/cm^3$$

$$n_e(30K) = \frac{2}{\lambda^3} e^{-E_F(30K)/k_BT} \approx 10^{15}/cm^3$$

For holes, since $E_g \sim 1.4 eV$

$k_B T \sim 25 meV$ for $300K$

and $E_F \sim 0.1 eV$ below E_c or $1.3 eV$ above E_v

$\Rightarrow n_{hole} \approx 0$ at $300K$
and at $30K$.

d) For the split-off band, the concentration of holes $\sim e^{-\Delta/k_B T}$ where $\Delta \sim 0.3 eV = 300 meV$

and $k_B T \sim 25 meV$ at $300K$

so it's justified to neglect terms in e^{-10}.

e) In the donor doping case, the donor band may lie very close to E_c from below. Similarly, the acceptor band may lie below E_v but above the split-off band. The population of holes $\propto e^{-|\Delta - E_F|/k_B T}$ and may not be necessarily small.

(f) The radius of the first Bohr orbit is increased by $\epsilon \cdot \frac{m}{m_e}$ over $0.53 Å$ (for free Hydrogen atom); In this case, $15 \times \frac{1}{0.07} \times 0.53 Å = 113.6 Å$, which is a large radius. So donor orbits overlap at relatively low donor concentrations. With appreciable overlap. "an impurity band" is formed from the donor states.

By Mott estimation (see Kittel P. 268.), $a_c \leq 4.5a_0 \sim 4.5 \times 15 \times 0.53\,\text{Å}$
$\sim 36\,\text{Å}$,

$\Rightarrow$ approximately for $N_d \sim 1/(36\text{Å})^3 \sim 10^{19}/\text{cm}^3$, we expect the donor electrons to form an impurity band.

The semi-conductor can conduct in the impurity band by electrons hopping from donor to donor.

The process of impurity band conduction sets in at lower donor concentration levels if there are also some acceptor atoms present, so that some of the donors are always ionized.

(f). Vegard's law doesn't apply to indirect gap - direct gap mixed materials since the conduction band minima of each material moves independantly of the other.

SOLUTION SET FOR PROBLEM SET #2

4. In silicon we will form pockets at the Δ-point, midway between the Γ and X points. The dispersion relation is given as

$$E(\vec{k}) = \frac{\hbar^2 k_\ell^2}{2m_\ell} + \frac{\hbar^2(k_{t_1}^2 + k_{t_2}^2)}{2m_t}$$

thus giving ellipsoidal pockets.

a) For one such pocket we have

$$\overleftrightarrow{\sigma} = n_1 e^2 \tau \left(\frac{\overleftrightarrow{I}}{m^*}\right) = n e^2 \tau \begin{pmatrix} 1/m_t & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_\ell} \end{pmatrix}$$

We now can calculate $\vec{J} = \vec{J}(\vec{E})$ and find ~~the magnitude~~ σ

Thus $\quad \vec{J}\{\vec{E} \parallel 001\} = \overleftrightarrow{\sigma} \cdot \vec{E} = n e^2 \tau \begin{pmatrix} \frac{1}{m_t} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_\ell} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ E \end{pmatrix}$

$$\vec{J} = \frac{n e^2 \tau}{m_\ell} E \hat{z}$$

$$\vec{J} = \frac{n e^2 \tau}{m_\ell} \vec{E} \qquad\qquad \text{Let } \sigma_0 = \frac{n e^2 \tau}{m_0}$$

$$\sigma_{001} = \frac{n e^2 \tau}{m_\ell} = \sigma_0 \left(\frac{m_0}{m_\ell}\right)$$

$$\sigma_{001} = \frac{(10^{18}\,\mathrm{cm}^{-1})(4.8\times 10^{-10}\,\mathrm{esu})(10^{-14}\,\mathrm{sec})}{(0.98)(9.1\times 10^{-28}\,\mathrm{g})}$$

$$\sigma_{001} = 2.6 \times 10^{12} \ \frac{esu^2\,sec}{cm^3\,g}$$

$$\sigma_{001} = 2.87\ (\Omega\cdot cm)^{-1}$$

b. For $\vec{E} \parallel (111)$

$$\vec{J} = \overleftrightarrow{\sigma} \cdot \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} E$$

$$\vec{J} = \frac{ne^2\tau}{\sqrt{3}} \left(\frac{1}{m_t}\hat{x} + \frac{1}{m_t}\hat{y} + \frac{1}{m_\ell}\hat{z} \right) E$$

We will measure $\vec{j}$ along $\vec{E}$, or $j_{111} = \frac{ne^2\tau}{3}\left(\frac{2}{m_t} + \frac{1}{m_\ell}\right)E$

$$j_{111} = \frac{\sigma_0}{3}\left[2\left(\frac{m_0}{m_t}\right) + \left(\frac{m_0}{m_\ell}\right)\right]E$$

yielding

$$j_{111}/E = \sigma_{111} = \frac{\sigma_0}{3}\left(\frac{2}{0.19} + \frac{1}{0.98}\right)$$

$$\sigma_{111} = 10.8\ (\Omega\cdot cm)^{-1}$$

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c. For $\vec{E} \parallel (210)$ $\quad \vec{E} = \frac{1}{\sqrt{5}}(2\hat{x} + \hat{y})E$

(EXTRA)

$$\vec{J} = \frac{ne^2\tau}{\sqrt{5}} \begin{pmatrix} \frac{1}{m_t} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_\ell} \end{pmatrix} \begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix} E$$

$$\vec{J} = \frac{ne^2\tau}{\sqrt{5}} \left(\frac{2}{m_t}\hat{x} + \frac{1}{m_t}\hat{y} + 0\cdot\hat{z} \right) E$$

$$j_{210} = \frac{ne^2\tau}{\sqrt{5}} \cdot \frac{1}{\sqrt{5}} \frac{5}{m_t} E = \frac{ne^2\tau}{m_t} E \implies \sigma_{210} = \sigma_0\left(\frac{m_0}{m_t}\right)$$

$$\sigma_{210} = 14.4\ (\Omega\cdot cm)^{-1}$$

2. Now we must sum 6 pockets, each containing $\frac{n}{6}$ electrons/cm^3

$$\overleftrightarrow{\sigma}_T = \sum_{i=1}^{6} \overleftrightarrow{\sigma}_i = ne^2\tau \sum_{i=1}^{6}{}' \begin{pmatrix} \frac{1}{m_t}, \frac{1}{m_l} & 0 & 0 \\ 0 & \frac{1}{m_t}, \frac{1}{m_l} & 0 \\ 0 & 0 & \frac{1}{m_t}, \frac{1}{m_l} \end{pmatrix}$$

$$\overleftrightarrow{\sigma}_T = ne^2\tau \begin{pmatrix} \frac{4}{m_t} + \frac{2}{m_l} & 0 & 0 \\ 0 & \frac{4}{m_t} + \frac{2}{m_l} & 0 \\ 0 & 0 & \frac{4}{m_t} + \frac{2}{m_l} \end{pmatrix}$$

$$\overleftrightarrow{\sigma}_T = 2ne^2\tau \left(\frac{2}{m_t} + \frac{1}{m_l}\right) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Hence, $\sigma_{001} = 64.9\,(\Omega.\text{cm})^{-1} = \sigma_{111}$