**Problem 4. (25 Points)**

**A. (15 Points)** Consider a mystery crystal at T=300 K in which $N_D = 4 \times 10^{13}$ $cm^{-3}$ and $N_A = 7 \times 10^{13}$ $cm^{-3}$. Assume $n_i = 1.5 \times 10^{13}$ $cm^{-3}$ and complete dopant ionization. Calculate the electron AND hole concentration.

$$n_o + N_A = P_o + N_D$$

$N_D < N_A$ so crystal is p-type → solve for majority carrier $P_o$

$$P_o + (N_D - N_A) = n_o = n_i^2 / P_o$$

$$P_o^2 + P_o(N_D - N_A) - n_i^2 = 0$$

$$P_o = \frac{-(N_D - N_A) \pm \sqrt{(N_D - N_A)^2 + 4n_i^2}}{2}$$

$$= \frac{3\times10^{13} \pm \sqrt{9\times10^{26} + 4(2.25\times10^{26})}}{2} = \frac{3\times10^{13} \pm 3\times10^{13}\sqrt{2}}{2}$$

$$= \frac{3\times10^{13}(1+\sqrt{2})}{2} = 3.62\times10^{13}\ cm^{-3}$$

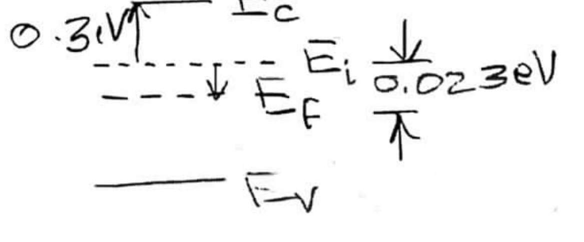
$$n_o = \frac{n_i^2}{P_o} = \frac{2.25\times10^{26}}{3.62\times10^{13}} = 6.2\times10^{12}\ cm^{-3}$$

**B. (10 Points)** Assume this mystery crystal has a band gap of 0.6 eV. Calculate the position of the Fermi level with respect to the intrinsic Fermi level ($E_i$) and draw the band diagram showing the Fermi level position quantitatively and to scale. $k_BT = 0.0259$ eV at 300 K.

$$P_o = n_i e^{(E_i - E_F)/k_BT}$$

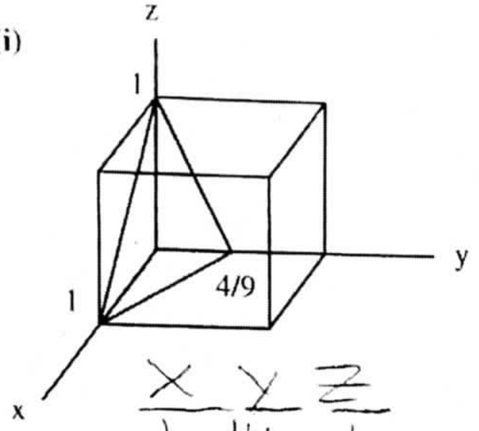
$$E_i - E_F = k_BT \ln(P_o/n_i) = 0.0259eV \ln \frac{3.6\times10^{13}}{1.5\times10^{13}}$$

$$= 0.88\,(0.0259eV) = 0.023eV \text{ below } E_i$$



**C. (10 Points)** Determine the Miller indices for the planes in the cubic unit cells below:

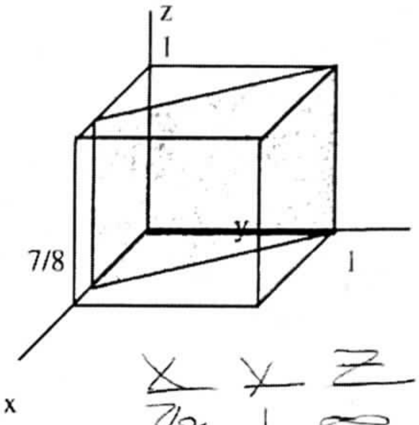
(i)




| X | Y | Z |
|---|---|---|
| 1 | 4/9 | 1 |
| 1/1 | 9/4 | 1 |
| 4 | 9 | 4 |

(494)

(ii)




| X | Y | Z |
|---|---|---|
| 7/8 | 1 | $\infty$ |
| 8/7 | 1 | 0 |
| 8 | 7 | 0 |

(870)

**D. (10 Points)** An elemental crystal with body centered lattice structure has a density of 7.19 g/cm$^3$, and an atomic radius of 0.125 nm. What is its atomic weight?

BCC unit cell has 2 atoms/u.c. (1 center + $\frac{1}{8}$ × 8 corners)

$$\rho = \frac{n}{V_c}\frac{A}{N_A} \rightarrow A = \frac{\rho V_c N_A}{n}$$

$$A = \frac{(7.19\ gm/cm^3)(6.02\times10^{23}\ atoms/mol)\,a^3\ cm^3}{2\ atoms}$$

$$\sqrt{3}\,a = 4R$$
$$a = \frac{4}{\sqrt{3}} R$$

$$a = \frac{4(0.125\,nm)}{1.732} = 0.289\ nm$$
$$= 2.89\times10^{-8}\ cm$$

$$A = \frac{7.19\times6.02\times10^{23}\times24.06\times10^{-24}}{2}\ gm/mol$$
$$= 520.7\times10^{-1} = 52.07\ gm/mol$$

**E. (5 Points)** What is its atomic packing fraction?

$$2\ atoms/unit\ cell = \frac{4\pi R^3}{3}\times2 = \frac{8\pi R^3}{3}$$

$$unit\ cell = a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

$$APF = \frac{8\pi R^3}{3} \Big/ \frac{64R^3}{3\sqrt{3}} = \frac{\pi\sqrt{3}}{8} = 0.68$$