STATE UNIVERSITY OF NEW YORK AT BUFFALO

Department of Mechanical and Aerospace Engineering

MEA 589 Diffraction, Microscopy and Spectroscopy Techniques

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HOMEWORK NO. 1

S O L U T I O N

Problem 1

(a) 8

(b) 6(1/2) + 8(1/8) = 3 + 1 = 4

(c) 4

(d) 8

(e) F cubic Bravais lattice

(f) 2 Na^+ and 1 O^{2-} in the basis

(g) Na^+ and O^{2-} touch each other along the body diagonal of the cube. Thus,

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

(h) $$\text{Density} = \frac{\text{Mass of unit cell}}{\text{Volume of unit cell}}$$

Mass of unit cell = 4 (16 amu) + 8 (23 amu)

= 248 amu

$$= \frac{248 \text{ amu}}{6.02 \times 10^{23} \text{ amu/g}}$$

$= 4.12 \times 10^{-22}$ g

From the periodic table,

$$r = 0.95 \text{ Å}$$

$$R = 1.40 \text{ Å}$$

Hence, according to the result of (g),

$$a = \frac{4}{\sqrt{3}}(r + R) = 5.427 \text{ Å}$$

Volume of unit cell = $a^3 = (5.427 \text{ Å})^3 = 1.598 \times 10^2 \text{ Å}^3 = 1.598 \times 10^{-22} \text{ cm}^3$

$$\text{Density} = \frac{4.12 \times 10^{-22} \text{ g}}{1.598 \times 10^{-22} \text{ cm}^3} = \underline{\underline{2.58 \text{ g/cm}^3}}$$

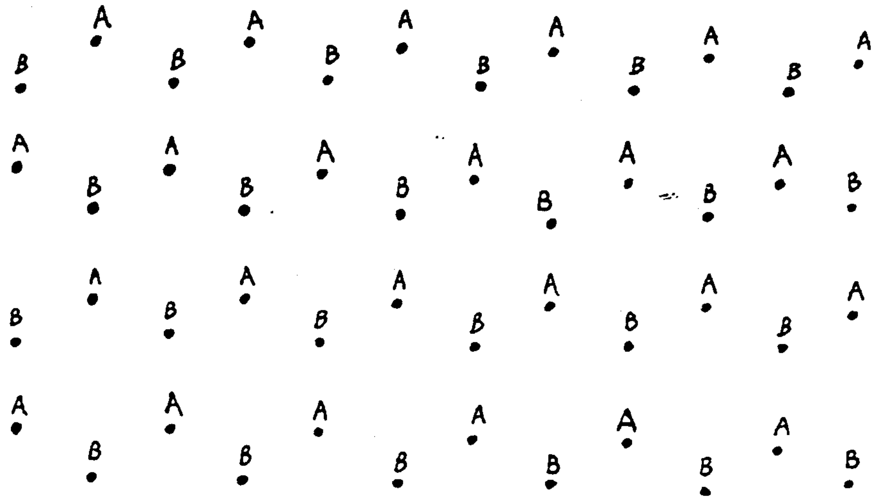
Problem 2

(a) 1

(b) 6 (1/3) + 1 = 2 + 1 = 3

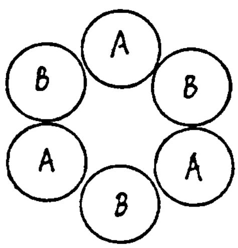
(c) parallelogram

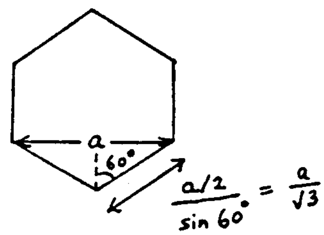
(d)



(e) 3

(f)





$$\frac{a}{\sqrt{3}} = 2r$$

Problem 3

For FCC,

$$a = \frac{4r}{\sqrt{2}}$$

For lead, r = 1.750 Å,

Thus

$$a = \frac{4}{\sqrt{2}} (1.750 \text{ Å})$$

$$= 4.950 \text{ Å}$$

Volume of the unit cell $= a^3$

$= (4.950\ \text{Å})^3$

$= \underline{\underline{121\ \text{Å}^3}}$

Problem 4

For the HCP structure,

$a = 2r.$

For Mg, $r = 1.61$ Å (given).

Thus, $a = 2\ (1.61\ \text{Å}) = 3.22\ \text{Å}$

Since $\frac{c}{a} = 1.62$,

$c = 1.62\ a = 1.62\ (3.22\ \text{Å}) = 5.21\ \text{Å}.$

Consider the hexagonal unit cell of the HCP structure.
No. of atoms per unit cell = 6

Volume of a unit cell $= \frac{3}{2}\sqrt{3}\ a^2\ c$

$$\text{Density} = \frac{\text{Mass of atoms in a unit cell}}{\text{Volume of a unit cell}}$$

$$= \frac{6\left(\frac{24.31\ \text{g}}{6.02 \times 10^{23}}\right)}{\frac{3}{2}\sqrt{3}\ (3.22\ \text{Å})^2\ (5.21\ \text{Å})}$$

$$= \underline{\underline{1.73\ \text{g/cm}^3}}$$

Problem 5

The electron energy levels for a copper atom are $E_K = -8982$ eV, $E_L = -933$ eV, and $E_M = -75$ eV. Calculate (a) the K_α photon energy, (b) the K_β photon energy, (c) the L_α photon energy, (d) the KLL Auger electron energy, and (e) the LMM Auger electron energy.

(a) $E_{K_\alpha} = |E_K - E_L| = |-8982\text{eV} - (-933\text{eV})| = \underline{\underline{8049\text{eV}}}$

(b) $E_{K_\beta} = |E_K - E_M| = |-8982\text{eV} - (-75\text{eV})| = \underline{\underline{8907\text{eV}}}$

(c) $E_{L_\alpha} = |E_L - E_M| = |-933\text{eV} - (-75\text{eV})| = \underline{\underline{858\text{eV}}}$

(d) $E_{KLL} = |E_K - E_L| - |E_L| = 8049\text{eV} - 933\text{eV} = \underline{\underline{7116\text{eV}}}$

(e) $E_{LMM} = |E_L - E_M| - |E_M| = 858\text{eV} - 75\text{eV} = \underline{\underline{783\text{eV}}}$

Problem 6

The K shell electron energy for nickel is $E_K = -8333$ eV and the wavelengths of the NiK_α and NiK_β photons are 0.1660 nm and 0.1500 nm, respectively. (a) Draw an energy-level diagram for a nickel atom. Calculate (b) the KLL and (c) the LMM Auger electron energies for nickel.

(a) $|E_K - E_L| = E_{K_\alpha} = \dfrac{hc}{\lambda_{K_\alpha}}$

$$= \frac{(0.6626\times10^{-33}\,J\cdot s)(0.2998\times10^{9}\,m/s)}{(0.1660\times10^{-9}\,m)(1\,J/6.242\times10^{18}\,eV)}$$

$= 7470\ eV$

$\therefore\ E_L = -8333\,eV + 7470\,eV = -863\,eV$

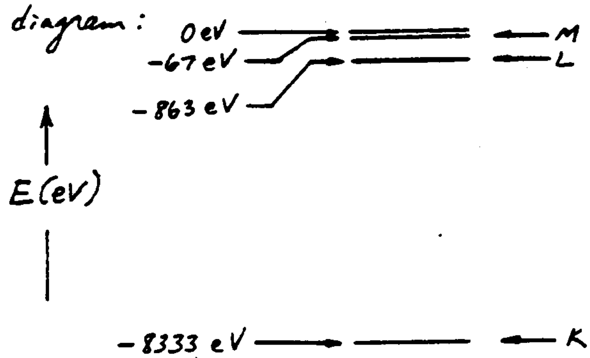
$|E_K - E_M| = E_{K_\beta} = \dfrac{hc}{\lambda_{K_\beta}}$

$$= \frac{(0.6626\times10^{-33}\,J\cdot s)(0.2998\times10^{9}\,m/s)}{(0.1500\times10^{-9}\,m)(1\,J/6.242\times10^{18}\,eV)}$$

$= 8266\ eV$

$\therefore\ E_M = -8333\,eV + 8266\,eV = -67\,eV$

giving the diagram:



(b) $E_{KLL} = |E_K - E_L| - |E_L|$

$= 7470\,eV - (863\,eV) = \underline{\underline{6607\,eV}}$

(c) $E_{LMM} = |E_L - E_M| - |E_M|$

$= |-863\,eV - (-67\,eV)| - |-67\,eV|$

$= 796\,eV - 67\,eV = \underline{\underline{729\,eV}}$