

Bragg's Law	Inter-planar Spacing	Hydrogen Like Spectra ( $R = 1.097 \times 10^7 \text{ m}^{-1}$ )
$2d_{hkl} \sin\theta = n\lambda$	$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$	$\frac{1}{\lambda} = RZ^2 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$

1. The voltage across an X-ray tube is 47.0 kV. The tungsten ( $Z = 74$ ) is the target in the X-ray tube. Determine (a) the tube's cutoff wavelength (b) the wavelength of the  $K_\alpha$  and  $L_\beta$  - ray lines emitted by the tungsten target.

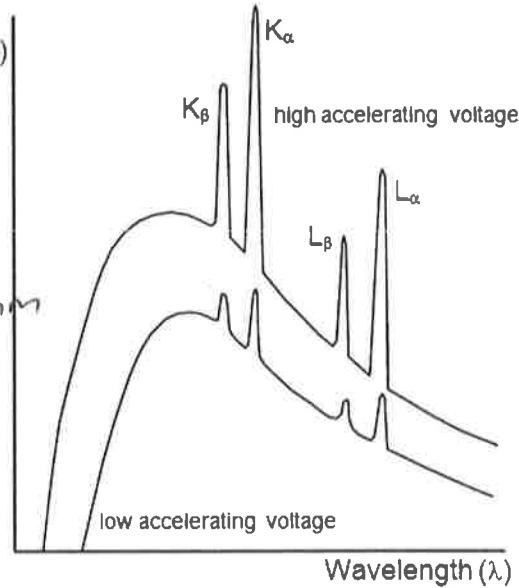
(a)  $E = \frac{hc}{\lambda} = eV$

$\lambda = \frac{hc}{eV}$

$\lambda = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19} \times 47 \times 10^3}$

$\lambda = 0.264 \times 10^{-10} \text{ m} = 0.0264 \text{ nm}$

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(b)  $\frac{1}{\lambda_{K\alpha}} = R(Z-1)^2 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$   
 $= R(74-1)^2 \left( \frac{1}{1^2} - \frac{1}{2^2} \right)$

$\frac{1}{\lambda_{K\alpha}} = 1.097 \times 10^7 \times 73^2 \times \left( 1 - \frac{1}{4} \right) = 4384.4 \times 10^7$

$\lambda_{K\alpha} = \frac{1}{4384.4 \times 10^7} = 2.280 \times 10^{-4} \times 10^{-7} \text{ m}$   
 $= 2.28 \times 10^{-11} \text{ m} = 0.0228 \text{ nm}$

$\frac{1}{\lambda_{L\beta}} = R(Z-7.4)^2 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$

$= 1.097 \times 10^7 \times (74-7.4)^2 \left( \frac{1}{2^2} - \frac{1}{4^2} \right) = 912.3 \times 10^7$

$\lambda_{L\beta} = \frac{1}{912.3 \times 10^7} = 0.001096 \times 10^{-7} \text{ m}$

$\lambda_{L\beta} = 0.1096 \text{ nm}$

Bragg's law for X-ray diffraction:

$$2d_{hkl} \sin \theta = n\lambda \quad d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Additional Conditions: BCC:  $h+k+l$ =even      FCC:  $h,k,l$  either odd or even

2. The  $2\theta$  values in degrees for diffraction peaks are given below for a metal with cubic structure, using X-rays of wavelength 0.1542 nm: 37.21, 43.23, 62.86, 75.31, 79.32.

(a) Derive an expression for

$$\frac{\sin^2 \theta}{h^2 + k^2 + l^2}$$

$$2 \frac{a}{\sqrt{h^2 + k^2 + l^2}} \cdot \sin \theta = \lambda$$

$$\frac{\sin^2 \theta}{h^2 + k^2 + l^2} = \frac{\lambda^2}{4a^2}$$

(b) Complete the table below.

(c) Determine the crystal structure. (FCC)

(d) Determine the lattice constant.

(e) Determine the ionic radius.

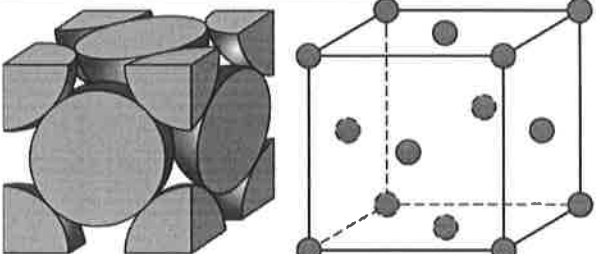
$2\theta$ (deg.)	$\theta$	$\sin^2 \theta$	Normalize	Clear Fractions	$h^2+k^2+l^2$	(hkl)	$\frac{\sin^2 \theta}{h^2 + k^2 + l^2}$
37.21	18.605	0.102	1	3	3	(111)	0.034
43.23	21.615	0.134	1.31	4	4	(200)	0.034
62.86	31.43	0.272	2.67	8	8	(220)	0.034
75.31	37.655	0.273	3.66	11	11	(311)	0.034
79.32	39.66	0.407	3.99	12	12	(222)	0.034

FCC

$$\frac{\lambda^2}{4a^2} = 0.034$$

$$a = 0.418 \text{ nm} \rightarrow \sqrt{2} a = 4R$$

$$R = 0.148 \text{ nm}$$

$\rho_{ave} = \frac{100}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2}}$	$A_{ave} = \frac{100}{\frac{C_1}{A_1} + \frac{C_2}{A_2}}$	
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3. Silver and palladium both have the FCC crystal structure, and Pd forms a substitutional solid solution for all concentrations at room temperature. Compute the unit cell edge length for a 65 wt% Ag–35 wt% Pd alloy. The room-temperature density of Pd is 12.02 g/cm<sup>3</sup>, and its atomic weight is 106.4 g/mol. The room-temperature density of Ag is 10.49 g/cm<sup>3</sup>, and its atomic weight is 107.9 g/mol.

$$\rho_{ave} = \frac{100}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2}} = \frac{100}{\frac{65}{10.49} + \frac{35}{12.02}} = 10.98 \frac{\text{g}}{\text{cm}^3}$$

$$A_{ave} = \frac{100}{\frac{C_1}{A_1} + \frac{C_2}{A_2}} = \frac{100}{\frac{65}{107.9} + \frac{35}{106.4}} = 107.4 \frac{\text{g}}{\text{mol}}$$

$$V = \frac{M}{\rho} = \frac{4 \cdot A_{ave} / N_A}{10.98}$$

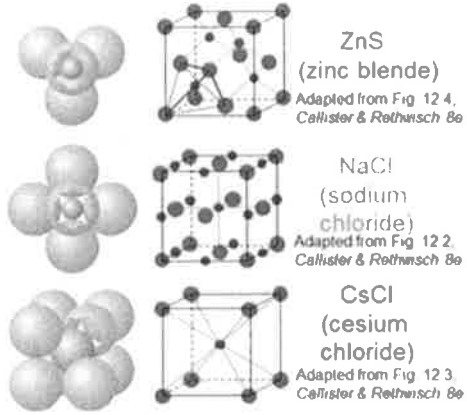
$$a^3 = \frac{4 \cdot 107.4}{10.98 \times 6.022 \times 10^{23}}$$

$$a = \left[ \frac{4 \times 107.4}{10.98 \times 6.022 \times 10^{23}} \right]^{1/3} = 4.02 \times 10^{-8} \text{ cm}$$

$a = 0.402 \text{ nm}$

**Table 12.3 Ionic Radii for Several Cations and Anions  
(for a Coordination Number of 6)**

Cation	Ionic Radius (nm)	Anion	Ionic Radius (nm)	$\frac{r_{\text{cation}}}{r_{\text{anion}}}$
$\text{Al}^{3+}$	0.053	$\text{Br}^-$	0.196	0.225-0.414
$\text{Ba}^{2+}$	0.136	$\text{Cl}^-$	0.181	
$\text{Ca}^{2+}$	0.100	$\text{F}^-$	0.133	
$\text{Cs}^+$	0.170	$\text{I}^-$	0.220	
$\text{Fe}^{2+}$	0.077	$\text{O}^{2-}$	0.140	0.414-0.732
$\text{Fe}^{3+}$	0.069	$\text{S}^{2-}$	0.184	
$\text{K}^+$	0.138			
$\text{Mg}^{2+}$	0.072			
$\text{Mn}^{2+}$	0.067			0.732-1.0
$\text{Na}^+$	0.102			
$\text{Ni}^{2+}$	0.069			
$\text{Si}^{4+}$	0.040			
$\text{Ti}^{4+}$	0.061			



4. On the basis of ionic charge and ionic radii given in Table 12.3, predict crystal structures for the following materials:

- (a) CsI
- (b) NiO
- (c) KI
- (d) NiS

Justify your selections.

(a)  $\text{CsI}$   $\frac{r_{\text{Cs}^+}}{r_{\text{I}^-}} = \frac{0.170}{0.220} = 0.773 \rightarrow \text{CsCl structure}$

(b)  $\text{NiO}$   $\frac{r_{\text{Ni}^{2+}}}{r_{\text{O}^{2-}}} = \frac{0.069}{0.140} = 0.493 \rightarrow \text{NaCl structure}$

(c)  $\text{KI}$   $\frac{r_{\text{K}^+}}{r_{\text{I}^-}} = \frac{0.138}{0.220} = 0.627 \rightarrow \text{NaCl structure}$

(d)  $\text{NiS}$   $\frac{r_{\text{Ni}^{2+}}}{r_{\text{S}^{2-}}} = \frac{0.069}{0.184} = 0.375 \rightarrow \text{Zincblende structure}$

$$R = \frac{\rho l}{A}$$

the resistivity of aluminum is  $2.7 \times 10^{-8} \Omega\text{-m}$

$$V = IR \quad J = I/A \quad E = V/L$$

5. (a) Compute the resistance of an aluminum wire 5 mm (0.20 in.) in diameter and 5 m (200 in.) in length.

$$R = \frac{\rho l}{A} = \frac{2.7 \times 10^{-8} \times 5}{\pi \times (2.5 \times 10^{-3})^2} = 6.89 \times 10^{-3} \Omega$$

(b) What would be the current flow if the potential drop across the ends of the wire is 0.04 V?

$$I = \frac{V}{R} = \frac{0.04}{6.89 \times 10^{-3}} = 5.81 \text{ A}$$

(c) What is the current density?

$$J = \frac{I}{A} = \frac{5.81}{\pi \times (2.5 \times 10^{-3})^2} = 2.96 \times 10^5 \text{ A/m}^2$$

(d) What is the magnitude of the electric field across the ends of the wire?

$$E = \frac{V}{L} = \frac{0.04}{5 \text{ m}} = 0.008 \text{ V/m}$$

$$\sigma = n|e|\mu_e + p|e|\mu_h$$

6. The following electrical characteristics have been determined for both intrinsic and p-type extrinsic indium phosphide (InP) at room temperature:

	$\sigma (\Omega\text{-m})^{-1}$	$n (m^{-3})$	$p (m^{-3})$
Intrinsic	$2.5 \times 10^6$	$3.0 \times 10^{13}$	$3.0 \times 10^{13}$
Extrinsic (n-type)	$3.6 \times 10^5$	$4.5 \times 10^{14}$	$2.0 \times 10^{12}$

Calculate electron and hole mobilities.

$$3.6 \times 10^5 = 4.5 \times 10^{14} \times 1.6 \times 10^{-19} \mu_e + 2 \times 10^{12} \times 1.6 \times 10^{-19} \mu_h$$

$$112.4 = 225 \mu_e + \mu_h \quad \text{--- (1)}$$

$$2.5 \times 10^6 = 3 \times 10^{13} \mu_e + 3 \times 10^{13} \times 1.6 \times 10^{-19} \mu_h$$

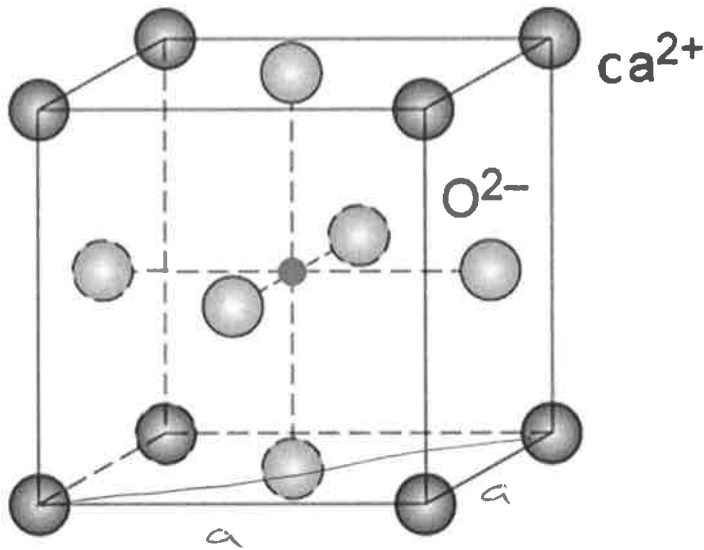
$$0.52 = \mu_e + \mu_h \quad \text{--- (2)}$$

① - ②

$$112.4 - 0.52 = 224 \mu_e \rightarrow \mu_e = 0.5 \frac{\text{m}^2}{\text{V}\cdot\text{s}}$$

$$\mu_h = 0.02 \frac{\text{m}^2}{\text{V}\cdot\text{s}}$$

7. Calculate the Density of  $\text{CaTiO}_3$ .



	$\text{Ti}^{4+}$	$\text{Ca}^{2+}$	$\text{O}^{2-}$
Radius	0.145 nm	0.100 nm	0.140 nm
Atomic weight	47.88 g	40.08 g	16 g

$$\sqrt{2} a = 2 R_{\text{Ca}} + 2 R_{\text{O}}$$

$$\sqrt{2} a = 2 \times 0.100 + 2 \times 0.140$$

$$a = \frac{2 \times 0.100 + 2 \times 0.140}{\sqrt{2}} = 0.339 \text{ nm}$$

$$\rho = \frac{m}{V} = \frac{3 A_{\text{O}} + 1 A_{\text{Ti}} + 1 A_{\text{Ca}}}{N_A \times (0.339 \times 10^{-7})^3} = \frac{3 \times 16 + 47.88 + 40.08}{6.022 \times 10^{23} \times (0.339 \times 10^{-7})^3}$$

$$\rho = 5.8 \frac{\text{g}}{\text{cm}^3}$$