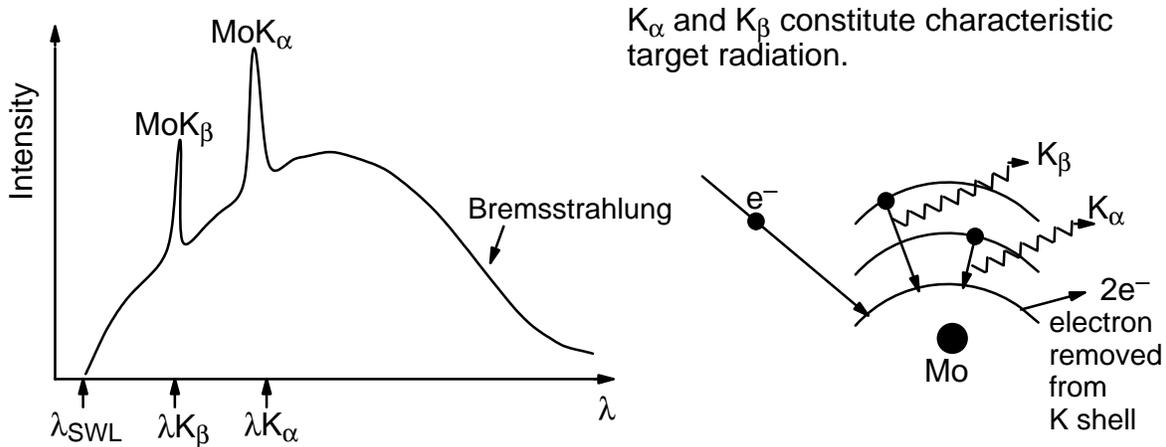


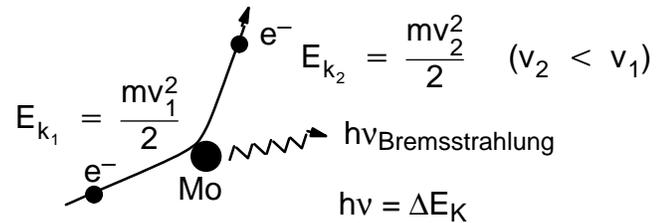
LN-5 IDLE MIND SOLUTIONS

1. (a) Schematic X-ray spectrum from a Mo target.



- (b) Characteristic Radiation:

After the vacancy is generated in the K shell, it may be filled by an electron transition from either the L shell (Mo K_{α} line) or from the M shell (Mo K_{β} line). Since the K_{β} transition is less likely to take place, its intensity on the spectrum is less than that of the K_{α} line.



Bremsstrahlung:

Bremsstrahlung constitutes conversion of E_{Kin} into $h\nu$, brought about by the deceleration of an electron upon close approach to the (potential energy barrier of the) nucleus. For an X-ray generator with E_{Kin} (electron) = eV, the shortest λ observable corresponds to a deceleration to $v=0$, or to the total conversion of eV into $h\nu$, thus $\lambda_{SWL} = hc/eV$.

$$(c) \quad \lambda_{SWL} = \frac{hc}{eV} = \frac{1.2 \times 10^{-6}}{V} \text{ (m)} = \frac{1.2 \times 10^4}{V} \text{ (\AA)} = \boxed{0.3 \times 10^{-10} \text{ m}}$$

2. In a BCC structure the smallest θ observable corresponds to the family of $\{110\}$ planes. Given $a = 10 \times 10^{-10}$ m, we find $d(110)$ to be:

$$d_{110} = \frac{a}{\sqrt{2}} = \boxed{7.07 \times 10^{-10} \text{ m}}$$

continued.

2. Continued.

Looking at a diffraction experiment we realize that $\theta_{(110)}$ will increase with increasing λ and can assume a maximum value of 90° for which $\sin\theta = 1$. For this maximum diffraction condition, the Bragg relation is reduced to:

$$\lambda = 2d_{(110)} = 2 \times 7.07 \times 10^{-10} \text{ m} = \boxed{14.14 \times 10^{-10} \text{ m}}$$

This finding means that any $\lambda > 14.14 \times 10^{-10} \text{ m}$ will not be able to lead to (110) diffraction.

3. To determine the lattice constant “a” for the metal requires identification of the Miller indices corresponding to the given diffraction angles – θ – which in turn first requires identification of the particular cubic system involved. To accomplish this identification, let us consider:

- (a) Selection rules:
- | | |
|--------|--|
| S.C. | All planes diffract |
| B.C.C. | Planes with $(h+k+l) = \text{even number}$ diffract |
| F.C.C. | Planes with only even or only odd (h,k,l) indices diffract |

- (b) The modified Bragg equation:

$$\frac{\lambda^2}{4a^2} = \frac{\sin^2\theta}{(h^2 + k^2 + l^2)} = \text{const.}$$

Taking (a) and (b), we find:

$$\text{SC} \quad \frac{\sin^2\theta_1}{1} = \frac{\sin^2\theta_2}{2} = \frac{\sin^2\theta_3}{3} = \frac{\sin^2\theta_7}{8} = \text{const.}$$

$$\text{BCC} \quad \frac{\sin^2\theta_1}{2} = \frac{\sin^2\theta_2}{4} = \frac{\sin^2\theta_3}{6} = \frac{\sin^2\theta_7}{14} = \text{const.}$$

$$\text{FCC} \quad \frac{\sin^2\theta_1}{3} = \frac{\sin^2\theta_2}{4} = \frac{\sin^2\theta_3}{8} = \text{const.}$$

(continued)

3. Continued.

- (a) The problem can now be reduced to finding the constant ratio, which requires finding the $\sin^2\theta$ values.

	<u>$\sin^2\theta$</u>
(1)	0.118
(2)	0.238
(3)	0.355
(4)	0.474
(5)	0.590
(6)	0.710
(7)	0.828

A quick look at the data suggests a BCC system since $\sin^2\theta_7$ is about 7 x $\sin^2\theta_1$.

We find:

$$\frac{\sin^2\theta_7}{14} = 0.059$$

and

$$\frac{\sin^2\theta_1}{2} = 0.059$$

A reminder: For the system to be SC (simple cubic):

$$\frac{\sin^2\theta_1}{1} = \frac{\sin^2\theta_7}{8} \quad (0.118 \neq 0.103)$$

For BCC the smallest θ value corresponds to the $\{110\}$ family. Therefore:

$$\lambda = 2d \sin \theta$$

$$d_{(110)} = \frac{\lambda}{2 \sin \theta_1} = \frac{1.541 \times 10^{-10}}{2 \times 0.344} = \boxed{2.24 \times 10^{-10} \text{ m}}$$

$$\text{We also have: } d_{(hkl)} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad \text{and} \quad a = d \times \sqrt{2}$$

$$\boxed{a = 3.17 \times 10^{-10} \text{ m}}$$

- (b) For a BCC system we find that atoms are in contact along the body diagonal:

$$a\sqrt{3} = 4r \quad \text{and} \quad \boxed{r = \frac{a\sqrt{3}}{4} = 1.37 \times 10^{-10} \text{ m}}$$

4. Cr: BCC; $r = 1.30 \times 10^{-10}$ m

In BCC systems the relationship between r and a is given by:

$$a\sqrt{3} = 4r \quad \text{and} \quad a = \frac{4r}{\sqrt{3}} = \frac{4 \times 1.30 \times 10^{-10}}{\sqrt{3}} = \boxed{3.00 \times 10^{-10} \text{ m}}$$

The first diffraction peak for BCC corresponds to $\{110\}$ planes; thus:

$$\lambda = 2d \sin\theta$$

$$\begin{aligned} \sin\theta_1 &= \frac{\lambda}{2d} \quad (d_{110} = \frac{a}{\sqrt{2}}) \\ &= \frac{\lambda}{\frac{2a}{\sqrt{2}}} = \frac{\lambda\sqrt{2}}{2a} = 0.3634 \end{aligned}$$

$$\boxed{\theta_1 = 21.3^\circ}$$

- Pd: FCC; $r = 1.37 \times 10^{-10}$ m

$$a\sqrt{2} = 4r \quad ; \quad a = 2\sqrt{2} r = 3.87 \times 10^{-10} \text{ m}$$

According to the selection rules, the first diffraction peak corresponds to the family of $\{111\}$ planes:

$$d_{(111)} = \frac{a}{\sqrt{3}} = \boxed{2.23 \times 10^{-10} \text{ m}}$$

$$\sin\theta_1 = \frac{\lambda}{2d} = 0.345$$

$$\boxed{\theta_1 = 20.2^\circ}$$

5. (a) While the diffraction angle for the (112) planes of Au can readily be calculated, this calculation serves no purpose since the selection rules prohibit diffraction at this set of planes! (FCC!)

5. Continued.

(b) Diffraction on {220} planes is encountered.

For FCC we have:

$$a\sqrt{2} = 4r \quad \text{and} \quad a = \frac{4r}{\sqrt{2}} = 2\sqrt{2}r = 4.13 \times 10^{-10} \text{ m}$$

$$\text{and} \quad d_{(200)} = \frac{a}{\sqrt{8}} = 1.46 \times 10^{-10} \text{ m}$$

$$\lambda = 2d \sin \theta$$

$$\sin \theta = \lambda / (2d) = 0.342$$

$$\theta = 20^\circ$$

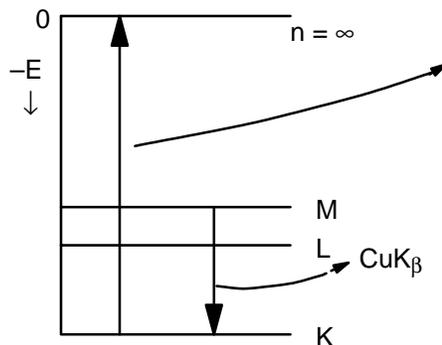
6. (a) The maximum energy (eV) of the electrons corresponds to the generation of λ_{SWL} as bremsstrahlung. Thus:

$$\lambda_{\text{SWL}} = \frac{hc}{eV} = \frac{1.24 \times 10^{-6}}{V} \text{ (m)} = 1.82 \times 10^{-10} \text{ m}$$

Since $\lambda_{\text{K}\alpha}$ is smaller than λ_{SWL} , it is clear that the energy of the incident electrons is insufficient to remove an electron from the K shell of Cu and thus no $\text{K}\alpha$ radiation can be generated.

(b) This question was answered in (a): $\lambda_{\text{SWL}} = 1.82 \times 10^{-10} \text{ m}$

(c) The answer to this question is **no!** This answer can be explained on the basis of an energy diagram.



energy required to remove an electron from the K shell! It can be seen that this energy (required to generate $\text{K}\beta$ radiation through the removal of an electron from the K shell) is significantly more than that associated with $\text{CuK}\beta$ radiation.

7. The system can only be BCC since $\sin^2\theta_7$ is $7 \times \sin^2\theta_1$; in SC systems the value of $\sin^2\theta$ after 0.600 would be 0.800!

8. The shortest wavelength emanated by a tube is given by:

$$\lambda_{\text{SWL}} = hc/eV \text{ (Bremsstrahlung)}$$

$$a = 3.26 \times 10^{-10} \text{ m}$$

BCC structure; first diffraction occurs on {110} planes:

$$d_{(110)} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{3.26}{\sqrt{2}} = \boxed{2.31 \text{ \AA}}$$

$$\lambda = 2d \sin\theta$$

$$\sin\theta \text{ is always } \leq 1, \text{ so } \lambda \leq 2d \leq \boxed{4.62 \times 10^{-10} \text{ m}}$$

$$\lambda_{\text{SWL}} = 4.62 \times 10^{-10} = hc/eV$$

$$V = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19} \times 4.62 \times 10^{-10}}$$

$$E = e \cdot V, \text{ so } V = \frac{4.25 \times 10^{-16} \text{ J}}{1.6 \times 10^{-19} \text{ eV/J}} = \boxed{2690 \text{ Volt}}$$

9. (a) SC: $\theta_{\{100\}}$

(b) BCC: $\theta_{\{110\}}$

(c) FCC: $\theta_{\{111\}}$

10. We determine the crystal system and from the constant ratio $[(\sin^2\theta)/(h^2+k^2+l^2) = \lambda^2/4a^2]$ we obtain "a" since λ is given. We look at θ_1, θ_2 (better $\sin^2\theta$) and, if necessary, at θ_7 .

	θ	$\sin\theta$	$\sin^2\theta$
(1)	13.70	0.2368	0.56092
(2)	15.89	0.2738	0.74962
(7)	36.62		

10. Continued.

The $\sin^2\theta$ values do not suggest BCC or SC structure, so that leaves FCC. We need only the first two ratios, but, for the exercise, let us identify all 9 diffraction lines!

	θ_B	$\sin\theta_B$	$\sin^2\theta_B/(h^2+k^2+l^2)$	ratio	
(1)	13.70	0.2368	0.05609/3	0.0187	(111)
(2)	15.89	0.2738	0.07496/4	0.0187	(200)
(3)	22.75	0.3867	0.1496/8	0.0187	(220)
(4)	26.91	0.4526	0.2048/11	0.0186	(311)
(5)	28.25	0.4733	0.2240/12	0.0187	(222)
(6)	33.15	0.5468	0.2990/16	0.0187	(400)
(7)	36.62	0.5965	0.3558/19	0.0187	(331)
(8)	37.60	0.6101	0.3723/20	0.0186	(420)
(9)	41.95	0.6685	0.4469/24	0.0186	(422)

$$\frac{\lambda^2}{4a^2} = 0.0187 \quad a = \sqrt{\frac{(1.54)^2}{4 \times 0.0187}} = 5.63\text{\AA} = \boxed{5.63 \times 10^{-10} \text{ m}}$$

A brief check:

$$\lambda = 2d_{(111)} \sin 13.70$$

$$\lambda = 2 \frac{a}{\sqrt{3}} \sin 13.70$$

$$a = \frac{1.54 \times \sqrt{3}}{2 \times 0.2368} = \boxed{5.63\text{\AA}}$$

11. First we determine $\lambda_{K\alpha}(\text{Cu})$. We also know that Ag crystallizes in an FCC lattice; thus the three smallest θ_B values are generated by the (111), (200), and (220) planes.

Using the Bragg relation, $\lambda = 2d_{(h,k,l)} \sin\theta_B$, we recognize that we have two unknowns: d ("a") and θ_B (to be determined).

$$\lambda = 2d_{(111)} \sin\theta_1 \quad d_{(111)} = \frac{a}{\sqrt{3}}$$

$$a = \sqrt[3]{\frac{4 \times 10.3 \times 10^{-6}}{6.02 \times 10^{23}}} = 4.09\text{\AA}$$

$$d_{(111)} = 2.36 \times 10^{-10} \text{ m}$$

$$10.3 \times 10^{-6} = (N_A/4)a^3$$

$$\theta_1 = \sin^{-1} \frac{1.54 \times 10^{-10}}{2 \times 2.36 \times 10^{-10}} = \boxed{19.04^\circ}$$

$$\theta_2 = \sin^{-1} \frac{1.54 \times 10^{-10}}{2 \times 2.045 \times 10^{-10}} = \boxed{22.1^\circ} \quad [d_{(200)} = a/\sqrt{4} = 2.045\text{\AA}]$$

$$\theta_3 = \sin^{-1} \frac{1.54 \times 10^{-10}}{2 \times 1.446 \times 10^{-10}} = \boxed{32.2^\circ} \quad [d_{(220)} = a/\sqrt{8} = 1.446\text{\AA}]$$

12. In any X-ray tube, the shortest wavelength of X-rays generated (regardless of the target material) will be: $\lambda_{\text{SWL}} = hc/eV$. Moreover, the "longest" wavelength still generating diffraction will do so with a $\theta_B \rightarrow 90^\circ$. Therefore, the limiting wavelength criterion is given by:

$$\boxed{\lambda_{\text{longest}} = 2d \sin 90 = 2d}$$

(continued)

12. Continued.

Potassium (K) has BCC structure; thus the smallest θ is associated with {110} diffraction (= the largest interplanar spacing):

$$\lambda_{\text{SWL}} = 2d_{(110)} = 2 \frac{a}{\sqrt{2}} = \frac{hc}{eV}$$

$$V = \frac{hc}{e \times 2 \frac{a}{\sqrt{2}}} \quad a = \sqrt[3]{\frac{2 \times 45.46 \times 10^{-6}}{6.02 \times 10^{23}}} = 5.32 \text{ \AA}$$

$$V = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19} \frac{2 \times 5.32 \times 10^{-10}}{\sqrt{2}}} = \boxed{1.65 \times 10^3 \text{ Volt}}$$

13. We first determine the lattice constant (a) for Au, and then the wavelength (λ_p) available for diffraction which, in conjunction with the Bragg relationship, will yield the diffraction angle for (220) planes:

Au: FCC; mol. vol. = 10.2 cm^3

$$a = \sqrt[3]{\frac{4 \times 10.2 \times 10^{-6}}{6.02 \times 10^{23}}} = \boxed{4.08 \times 10^{-10} \text{ m}}$$

Electrons accelerated by 45 kV will have a kinetic energy of:

$$E_{\text{Kin}} = 4.5 \times 10^4 \times 1.6 \times 10^{-19} \text{ J} = (mv^2)/2$$

For convenience, let us determine v , the velocity of the electrons, and insert the value into the deBroglie equation:

$$v = \sqrt{\frac{9 \times 10^4 \times 1.6 \times 10^{-19}}{9.1 \times 10^{-31}}} = 1.26 \times 10^8 \text{ m/s}$$

(we ignore relativistic effects)

$$\lambda_p = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 1.26 \times 10^8}$$

$$\boxed{\lambda_p = 5.8 \times 10^{-12} \text{ m}}$$

(a short λ , θ_B will certainly be small)

13. Continued.

$$\lambda_p = 2d_{(hkl)} \sin \theta = 2 \frac{a}{\sqrt{8}} \sin \theta = \frac{a}{\sqrt{2}} \sin \theta$$

$$\theta_B = \sin^{-1} \frac{\lambda_p}{\frac{a}{\sqrt{2}}} = \sin^{-1} \frac{5.8 \times 10^{-12} \times \sqrt{2}}{4.08 \times 10^{-10}}$$

$$\theta_B = 1.15^\circ$$

14. From the selection rules we recognize that the first diffraction peak in BCC systems is due to (110) planes.

For vanadium, $\bar{v}K_\alpha = 3/4 R(23-1)^2 = 3.98 \times 10^9 \text{ m}^{-1}$

and $\lambda K_\alpha = 2.51 \times 10^{-10} \text{ m}$

$$\lambda = 2d \sin \theta$$

$$d_{(110)} = \frac{2.51 \times 10^{-10}}{2 \sin 41.75} = 1.885 \times 10^{-10} \text{ m}$$

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$a = d_{(110)} \times \sqrt{2}$$

$$a = 2.66 \times 10^{-10} \text{ m}$$

15. First order diffraction refers to "n" in the Bragg equation being one.

$$\bar{v} \text{ Ag } K_\alpha = 3/4 R(46)^2 = 1.74 \times 10^{10} \text{ m}^{-1}$$

$$\lambda \text{ Ag } K_\alpha = 0.574 \times 10^{-10} \text{ m}$$

Fe = BCC structure

$$\lambda = 2d_{(110)} \sin \theta$$

$$\sin \theta = \frac{\lambda}{2d_{(110)}}$$

$$\theta = \sin^{-1} \frac{\lambda}{2d_{(110)}} = 8.15^\circ$$

16. Ta: BCC structure; the smallest θ is due to (110) reflections.

$$\lambda = 2d_{(110)} \sin\theta$$

To determine λ , we must know $d_{(110)}$ – that means “a”, the lattice constant.

For Ta:

$$1.09 \times 10^{-5} \text{ (m}^3\text{/mole)} = (N_A/2)a^3$$

$$a = \sqrt[3]{\frac{2 \times 1.09 \times 10^{-5}}{6.02 \times 10^{23}}} = 3.31 \times 10^{-10} \text{ m}$$

$$d_{(110)} = \frac{a}{\sqrt{2}} = 2.34 \times 10^{-10} \text{ m}$$

$$\lambda = 2 \times 2.34 \times 10^{-10} \times \sin 29.35$$

$$\lambda = 2.29 \times 10^{-10} \text{ m} ; \bar{\nu} = 4.36 \times 10^9 \text{ m}^{-1}$$

Taking the Moseley relationship, we have:

$$4.36 \times 10^9 = 3/4 R (Z-1)^2$$

$$(Z - 1) = \sqrt{\frac{4 \times 4.36 \times 10^9}{3R}} = 23$$

$$Z = 24$$

The unknown target material is **chromium (Cr)**.

17. (a) First, realize that the two lines nearest the undiffracted beam will be due to the same diffraction cone (use the 3.091 diffraction software if you need to convince yourself of this). **This cone will be due to {111} planes**, which have the widest spacing in the FCC structure, and thus have the smallest diffraction angle, 2θ .

(continued)

17. Continued.

- (b) The radius of the camera is 5 cm, so a separation of 7.8 cm between lines is an angle of $7.8/5$ radians = 1.56 radians = 89° . This separation represents twice the diffraction angle, so $2\theta = 44.5^\circ$, and $\theta_{111} = 22.25^\circ$.

$$d_{111} = \frac{\lambda_{\text{CuK}\alpha}}{2 \sin \theta_{111}} = \frac{1.54 \text{ \AA}}{2 \sin 22.25} = 2.034 \text{ \AA}$$

$$a = d_{111} \sqrt{3} = 3.52 \text{ \AA}$$

For the FCC structure: $a\sqrt{2} = 4r$, so $r = \frac{a\sqrt{2}}{4} = 1.24 \text{ \AA}$

18. We first determine λ_p for the electrons through the deBroglie relationship, $\lambda_p = h/(mv)$. This requires knowledge of v :

$$E_{\text{el}} = e \times V = (mv^2)/2 \quad v = \sqrt{\frac{2e \times V}{m}}$$

Thus:
$$\lambda_p = \frac{h}{m \sqrt{\frac{2e \times V}{m}}} = \frac{h}{\sqrt{2e \times V \times m}}$$

$$\lambda_p = 3.9 \times 10^{-12} \text{ m}$$

$\lambda = 2d_{(hkl)} \sin\theta$; to determine θ we must know $d_{(112)}$, given by $a/\sqrt{6}$. We must first determine the lattice constant (a) for gold (Au). From the P/T we get: molar volume = $10.2 \times 10^{-6} \text{ m}^3$; accordingly (Au = FCC):

$$10.2 \times 10^{-6} = \frac{6.02 \times 10^{23}}{4} \times a^3$$

$$a = \sqrt[3]{\frac{40.8 \times 10^{-6}}{6.02 \times 10^{23}}} = 4.08 \times 10^{-10} \text{ m}$$

We now find that:

$$d_{(112)} = \frac{4.08 \times 10^{-10}}{\sqrt{6}} = 1.66 \times 10^{-10} \text{ m}$$

$$\sin \theta = \frac{\lambda}{2d_{(hkl)}} = \frac{3.9 \times 10^{-12}}{2 \times 1.66 \times 10^{-10}} = 1.17 \times 10^{-2}$$

$$\theta = \sin^{-1} 1.17 \times 10^{-2} = 0.67^\circ$$

After you have determined θ , think for a moment! OK!? Selection rules tell you that diffraction on $\{112\}$ planes are destructively interfered with! No diffraction on $\{112\}$!

19. We first determine the crystal system, then (knowing λ) we determine a and obtain the asked for molar volume.

	$\frac{2\theta}{\text{°}}$	$\frac{\theta}{\text{°}}$	$\frac{\sin\theta}{\text{°}}$	$\frac{\sin^2\theta}{\text{°}}$
(a)	40.50°	20.25	0.3461	0.1198
(b)	58.60°	29.30	0.4894	0.2395
(c)	132.60°	66.30	0.9156	0.8384

We recognize $0.8384 = 7 \times 0.1198$; this means $(\sin^2\theta_7)/14 = (\sin^2\theta_1)/2 = \text{const.}$
The system is BCC.

$$\lambda = 2d_{(110)} \sin\theta_1 = 2 \frac{a}{\sqrt{2}} \sin\theta$$

$$a = \frac{\sqrt{2} \times 1.541 \times 10^{-10}}{2 \times 0.3461} = 3.15 \times 10^{-10} \text{ m}$$

$$\text{Molar volume} = N_A/2(a^3) = 9.4 \times 10^{-6} \text{ m}^3/\text{mole} = \mathbf{9.4 \text{ cm}^3/\text{mole}}$$

20. From information in the P/T we know the molar volume of Ag at 300K. This allows us to determine $\theta_{(111)}$ through the lattice constant. With the given $\Delta\theta$ we can obtain $\theta_{(111)}$ at 1073K (which is 800°C).

$$\text{At 300K: Molar Volume} = 10.3 \times 10^{-6} = N_A/4(a^3)$$

$$a = \sqrt[3]{\frac{4 \times 10.3 \times 10^{-6}}{6.02 \times 10^{23}}} = 4.09 \times 10^{-10} \text{ m}$$

$$d_{(111)} = \frac{4.09 \times 10^{-10}}{\sqrt{3}} = 2.361 \times 10^{-10}$$

$$\lambda = 2d_{(111)} \sin\theta$$

$$\theta_{(111)} = \sin^{-1} \frac{\lambda}{2d_{(111)}} = \sin^{-1} \frac{0.709 \times 10^{-10}}{2 \times 2.361 \times 10^{-10}} = 8.64^\circ$$

$$\text{At 800°C (1073K): } \theta_{(111)} = 8.64 - 0.11 = 8.53^\circ$$

(continued next page)

20. Continued:

Correspondingly:

$$d_{(111)} = \frac{\lambda}{2 \sin 8.53} = 2.34 \times 10^{-10} \text{ m} = \frac{a}{\sqrt{3}}$$

$$a = \sqrt{3} \times 2.39 \times 10^{-10} \text{ m} = 4.14 \times 10^{-10}$$

$$\text{Molar Volume} = N_A/4 \times a^3 = 10.7 \times 10^{-6} \text{ m}^3/\text{mole}$$

$$= \boxed{10.7 \text{ cm}^3/\text{mole}}$$

21. We recognize that the existence of (100) diffraction indicates a simple cubic system. After determining the lattice constant, we can obtain the central void dimension and answer the question.

Required: (100) diffraction = SC
SC structure: $d_{(100)} = a$

$$\lambda = 2d \sin \theta = 2a \sin \theta$$

$$a = \lambda / (2 \sin \theta)$$

(The way the question is phrased, it may not appear clear if 14.88° is θ . The diffraction expert would take $14.88^\circ = 2\theta$, but you may have a different idea. Both assumptions are taken as correct.) Accordingly:

$$(a) \quad 14.88^\circ = \theta_1 \quad ; \quad a = \frac{\lambda}{2 \sin 14.88} = \frac{1.541}{2 \times 0.257} = \boxed{3.0 \text{ \AA}}$$

$$(b) \quad 14.88^\circ = 2\theta_1 \quad ; \quad a = \frac{\lambda}{2 \sin 7.44} = \frac{1.541}{2 \times 0.129} = \boxed{5.95 \text{ \AA}}$$

In the SC system we have a central void; an atom in this location is bounded along the body diagonal by all eight atoms:

(continued next page)

21. Continued.

$$2r = a$$

$$a\sqrt{3} = 2r + 2R = a + 2R$$

$$2R = a\sqrt{3} - a = a(\sqrt{3} - 1)$$

$$R = a \frac{(\sqrt{3} - 1)}{2} = 0.366 a$$

For (a): $R = 0.366 \times 3.0 = 1.1 \text{ \AA}$

R = maximum radius for
interstitial atoms

For (b): $R = 0.366 \times 5.95 = 2.18 \text{ \AA}$

Since the maximum radius for interstitial atoms is 1.1 and 2.18 Å for (a) and (b) respectively, **an atom with $r = 1.08 \text{ \AA}$ can be accommodated** without lattice distortion in either crystal lattice.

22. In a BCC system, the first diffraction (smallest θ) occurs on {110} planes (see selection rules, LN5–11). Given the lattice constant ($a = 5.5 \text{ \AA}$), we find the $d_{(110)}$ spacing at

$$d_{(110)} = \frac{5.5}{\sqrt{2}} = 3.89 \text{ \AA}$$

In order to obtain {110} diffraction (maximum $\theta = 90^\circ$ and $\sin\theta = 1$), $\lambda \leq 2d$ must be satisfied.

Since no target material for the tube is indicated, we take the smallest λ available from the X-ray generator, λ_{SWL} :

$$\lambda_{\text{SWL}} = \frac{hc}{eV} = \boxed{10.3 \text{ \AA}}$$

$$2d = 3.89 \times 2 = 7.78 \text{ \AA}$$

We find $10.3 > 7.78$ and therefore **no diffraction cone can be generated by this particular powder with the available X-rays.**

23. Grind the material to powder and do a Debye–Scherrer diffraction with $\text{CuK}\alpha$ radiation (λ listed or calculated). If the film shows diffraction lines, the material is crystalline [the answer to (a)]. If the $\sin^2\theta$ values for the first and seventh lines yield a constant ratio for:

$$\frac{\sin^2\theta_1}{2} = \frac{\sin^2\theta_7}{14} = \text{const}$$

we are dealing with a BCC structure [answer to (b)]. We obtain the lattice constant through the Bragg equation:

$$\lambda = 2d_{(110)} \sin\theta_1 \quad [d_{(110)} = \frac{a}{\sqrt{2}}]$$

$$\lambda = \frac{2a}{\sqrt{2}} \sin\theta_1$$

$$a = \frac{\lambda\sqrt{2}}{2\sin\theta_1}$$

24. To solve the problem we first determine the longest wavelength still capable of causing diffraction. From the Bragg relation: $\lambda = 2d_{(hkl)} \sin\theta$. To get diffraction, θ may assume a maximum value of 90° ($\sin 90^\circ = 1$). Accordingly:

$$\lambda_{\text{max}} = 2d_{(hkl)}$$

In FCC systems the largest diffraction d is $d_{(111)}$:

$$\lambda_{\text{max}} = 2d_{(111)} = 2(a/\sqrt{3}) = \boxed{6.93\text{\AA}}$$

Using the Moseley relation we know that $\lambda_{\text{Cr}}(\text{K}\alpha) = 2.3\text{\AA}$. Therefore diffraction will take place if $\text{K}\alpha$ radiation is generated by a 1.5 kV accelerating potential, or if λ_{SWL} is equal or less than 6.93\AA !

$$\lambda_{\text{SWL}} = (hc)/eV = (12.4 \times 10^{-6})/V = 8.29 \times 10^{-10} \text{ m}$$

We recognize that $\lambda_{\text{SWL}} > \lambda_{\text{max}}$. **There cannot be any diffraction given the X-rays from a tube operated at $V = 1.5 \times 10^3$ Volt.**

25. From Moseley's law we know that $\lambda K_{\alpha} \propto 1/Z^2$. As a first approximation, by comparing $\text{Cu}K_{\alpha}$ and $\text{Mo}K_{\alpha}$, we therefore have:

$$\lambda \text{Mo}K_{\alpha} \cong 1.542 \left(\frac{29}{42} \right)^2 = 0.735 \text{ \AA}$$

Or, more accurately:

$$1.542 \left(\frac{29 - 1}{42 - 1} \right)^2 = 0.719 \text{ \AA}$$

(The listed value for λK_{α} (Mo) = 0.71 \AA)

Since in replacing a Cu target with a Mo target the resulting λK_{α} is decreased, it must be expected that the first diffraction peak will shift to a smaller θ !!

26. Vanadium is BCC. The largest diffracting d is $d_{(110)}$. From the Bragg relation, $\lambda = 2d_{(hkl)} \sin\theta$, we recognize that θ can go up to 90° ($\sin\theta = 1$) and the longest wavelength still giving diffraction is seen to be:

$$\lambda_{\max} = 2d_{(110)} = 2(a/\sqrt{2})$$

For vanadium:

$$\text{Mol. Vol.} = N_A/2 \times a^3$$

$$a = \sqrt[3]{\frac{2 \times 8.78 \times 10^{-6}}{6.02 \times 10^{23}}} = 3.08 \times 10^{-10} \text{ m}$$

$$\lambda_{\max} = 2 \frac{a}{\sqrt{2}} = \boxed{4.35 \times 10^{-10} \text{ m}}$$

27. Mo: $Z=42$; $K_{\alpha} \rightarrow (n_i=2; n_f=1)$; $\sigma=1$

$$\bar{\nu}_{K\alpha} = R(Z-1)^2 \left[\frac{1}{n_f^2} - \frac{1}{n_i^2} \right]$$

$$\bar{\nu}_{K\alpha} = 1.097 \cdot 10^7 \left[\frac{1}{\text{m}} \right] (42-1)^2 \left[\frac{1}{1^2} - \frac{1}{2^2} \right]$$

$$\bar{\nu}_{K\alpha} = 1.38 \cdot 10^{10} \text{m}^{-1}$$

$$\lambda_{K\alpha} = \frac{1}{\bar{\nu}_{K\alpha}} = \boxed{7.25 \cdot 10^{-11} \text{m}}$$

28. $\frac{1}{\lambda_{K\alpha}} = \bar{\nu}_{K\alpha} = R(Z-1)^2 \left[\frac{1}{n_f^2} - \frac{1}{n_i^2} \right]$

$$= R(Z-1)^2 \cdot \frac{3}{4}$$

$$(Z-1) = \sqrt{\frac{4}{3 \cdot \lambda \cdot R}} = 22$$

$Z = 23$ (Vanadium)

29. Ni = FCC; $n = 4$; AtWt = 58.7; $\rho = 8.9 \text{ g/cm}^3$

To get the longest wavelength diffracting in Ni – we look for diffracting planes with maximum spacing ($\{111\}$) and we operate at the maximum θ possible (90°)

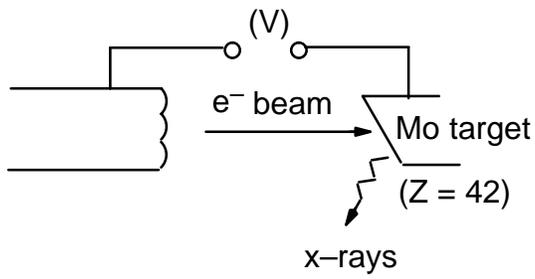
$$\lambda = 2d_{(111)} \sin \theta = 2 \frac{a}{\sqrt{3}} \sin 90^\circ = 2 \frac{a}{\sqrt{3}}$$

for nickel:

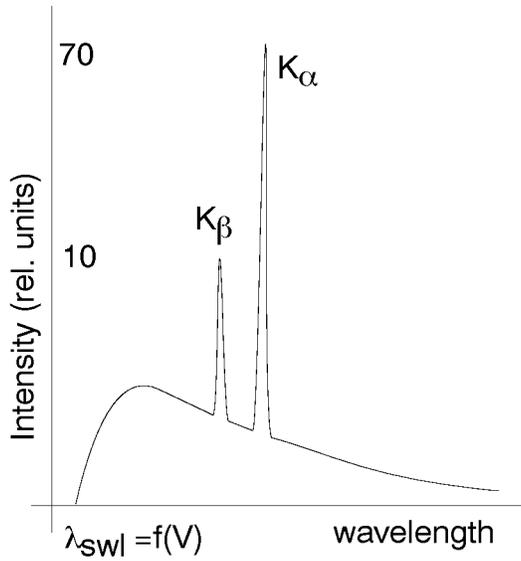
$$a(\text{Ni}) = \sqrt[3]{\frac{58.7 \cdot 4}{8.9 \cdot 6.02 \cdot 10^{23}}} = 3.52 \cdot 10^{-8} \text{cm} \cdot \frac{1 \text{m}}{100 \text{cm}} = 3.52 \cdot 10^{-10} \text{m}$$

$$\lambda = \frac{2 \cdot 3.52 \cdot 10^{-10}}{\sqrt{3}} = \boxed{4.06 \cdot 10^{-10} \text{m}}$$

30.



$$\lambda_{\text{SWL}} = \frac{hc}{eV} = \frac{1.24 \cdot 10^{-6} [\text{m}]}{\text{acc. Voltage}} = \frac{1.24 \cdot 10^{-6}}{5 \cdot 10^4} = \boxed{2.48 \times 10^{-11} \text{m}}$$



$$\lambda_{K_\alpha} = \frac{4}{3R(z-1)^2} = \boxed{7.23 \times 10^{-11} \text{m}}$$

how did I get λ_{K_α} ? $\bar{\nu}_{K_\alpha} = R(Z-1)^2 \frac{3}{4}$

$$\frac{1}{\lambda} = \bar{\nu} = \frac{4}{3R(Z-1)^2}$$

31. Electron diffraction makes use of the deBroglie relationship: $\lambda_p = \frac{h}{mv}$; we need $d_{(111)}$ that means we need, a , the lattice constant since: $d_{(111)} = \frac{a}{\sqrt{3}}$; the energy of the electron(s) is $eV_{(acc.)} = Mv^2/2$.

$$\lambda = 2d_{(111)} \sin \theta = \frac{2a}{\sqrt{3}} \sin \theta$$

$$\lambda_p = \frac{2a}{\sqrt{3}} \sin 6^\circ \quad a = \frac{\sqrt[3]{10.2 \cdot 10^{-6} \cdot 4}}{6.02 \cdot 10^{23}} = 4.08 \cdot 10^{-10} \text{m}$$

$$\lambda_p = \frac{2 \cdot 4.08 \cdot 10^{-10}}{\sqrt{3}} \cdot \sin 6^\circ = 4.92 \cdot 10^{-11} \text{m}$$

$$E_{el} = eV = \frac{mv^2}{2}$$

$$V = \frac{mv^2}{2e} ; \quad v = \frac{h}{m\lambda_p}$$

$$V = \frac{m}{2e} \cdot \frac{h^2}{m^2\lambda_p^2} = \frac{h^2}{2em\lambda_p^2} = \boxed{623.6 \text{ Volt}}$$

32. Let's make use of the data in problem (29): $a = 3.52 \times 10^{-10} \text{m}$; smallest acceleration potential means operating with the shortest λ achievable at a given acceleration potential:

$\lambda_{SWL} = \frac{1.24 \cdot 10^{-6}}{\text{Voltage}}$; the longest λ giving diffraction is at $\theta=90^\circ$ on planes with largest interplanar spacing ($\{111\}$).

$$\lambda_{SWL} = 2d_{(111)} \sin 90 = 2 \frac{a}{\sqrt{3}} = 4.06 \cdot 10^{-10} \text{m}$$

$$4.06 \cdot 10^{-10} = \frac{1.24 \cdot 10^{-6}}{V}$$

$$V = \frac{1.24 \cdot 10^{-6}}{4.06 \cdot 10^{-10}} = \boxed{3.06 \cdot 10^3 \text{ Volt}}$$

33. Operate at the unit cell level with the atomic volume:

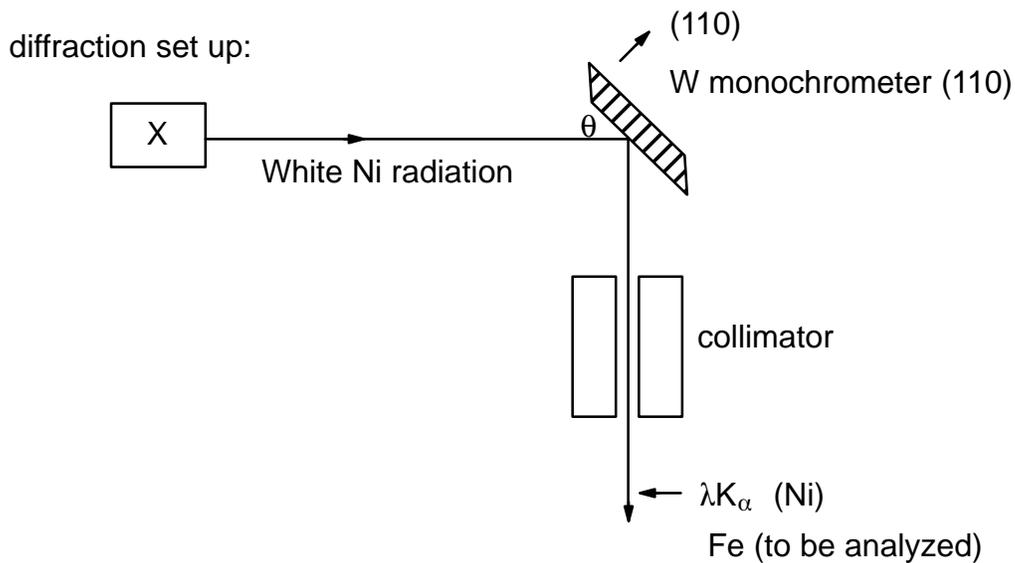
$$\text{Atomic Volume} = \frac{\text{At.wt}}{\rho} = \frac{N}{n} a^3 ; \text{ solve for At.wt.}$$

$$\frac{N}{n} \cdot a \cdot \rho = \frac{6.02 \cdot 10^{23}}{2} \cdot (0.316 \cdot 10^{-9})^3 \cdot 19.3 \cdot 10^6 \frac{\text{g}}{\text{m}^3}$$

$$\boxed{\text{At.wt} = 181.6 \text{g}}$$

(the factor of 10^6 associated with the density term accounts for the change of units from g/cm^3 to g/m^3)

34. A diffraction set-up is asked for with specification of conditions for achievement of λK_{α} . You have the choice of material to be used as monochromator; first determine λK_{α} (for Ni target) then decide on monochromator material. You could use Ni, or more conveniently, you just determine the atomic weight for tungsten (W; the W stands for Wolfram, the official german name) and you have its lattice constant.



$$\begin{aligned} \text{Ni}K_{\lambda} \quad \bar{\nu}K_{\lambda} &= 27^2 \cdot 1.097 \cdot 10^7 \cdot \frac{3}{4} \text{ (m}^{-1}\text{)} \\ &= 6.0 \times 10^9 \text{ (m}^{-1}\text{)} \end{aligned}$$

$$\lambda K_{\alpha} = 1.67 \times 10^{-10} \text{ m}$$

To isolate K_{α} from White Ni radiation we establish diffraction for

$$\lambda = 1.67 \times 10^{-10} \text{ m on (110) planes:}$$

$$\lambda K_{\alpha} = 2d_{(110)} \sin \theta = 2 \frac{a}{\sqrt{2}} \sin \theta$$

$$\sin \theta = \frac{\sqrt{2} \lambda K_{\alpha}}{2a} = \frac{\sqrt{2} \cdot 1.67 \cdot 10^{-10}}{2 \cdot 3.16 \cdot 10^{-10}} = 0.374$$

$$\theta = \sin^{-1} 0.374 = \boxed{21.9^{\circ}}$$

35. Determine the energy/photon then λ of radiation and use the Mosley relation to find Z the atomic #.

$$E_{\text{photon}} = 7.725 \cdot 10^8 \text{J} / 6.02 \cdot 10^{23} = 1.28 \cdot 10^{-15} \text{J/photon}$$

$$hc\bar{\nu} = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{1.28 \cdot 10^{-15}} = 1.55 \cdot 10^{-10} \text{m} \quad ; \quad \bar{\nu} = 6.45 \cdot 10^9 \text{m}^{-1}$$

$$\bar{\nu} = 6.45 \cdot 10^9 = (Z - 1)^2 R \frac{3}{4}$$

$$Z = \sqrt{\frac{4 \cdot 6.45 \cdot 10^9}{3 \cdot 1.097 \cdot 10^7}} + 1 = 28 + 1 = \boxed{29} \text{ (copper)}$$

36. This is a simple application of the Bragg relation: We determine “a” for Fe(BCC) and λK_{α} for Ni and insert:

λK_{α} (Ni) we know from Problem (34); it is $1.67 \times 10^{-10} \text{m}$ the lattice constant for

$$a = \sqrt[3]{\frac{2 \cdot 7.1 \cdot 10^{-6}}{6.02 \cdot 10^{23}}} = 2.87 \cdot 10^{-10} \text{m}$$

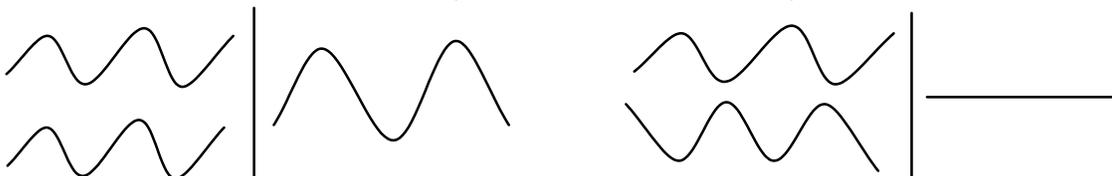
$$\text{Fe(BCC):} \quad \sin \theta = \frac{\sqrt{2} \cdot \lambda}{2 \cdot 2.87 \cdot 10^{-10}} = \frac{\sqrt{2} \cdot 1.67 \cdot 10^{-10}}{2 \cdot 2.87 \cdot 10^{-10}} = 0.411$$

$$\theta = \sin^{-1} 0.411 = 24.3^\circ$$

37. The unit cell is defined as a cell bounded by 3 sets of parallel planes which will fill all space when translated by multiples of the plane spacings. Cells that contain a total of one lattice point are called primitive cells, others are called “non-primitive” cells. Each cell is characterized by volume, shape and contents.

38. (a) close packed array of equal sized spheres (FCC) ————— 12
 (b) simple cubic structure (SC) ————— 6
 (c) body centered cubic lattice (BCC) ————— 8

39. If two or more parallel interacting waves are moving through a medium, the resultant wave function at any point is the algebraic sum of the wave functions of the individual waves. As a consequence of this “superposition” principle, the intensity of 2 waves that are coherent and have the same wavelength (coincidence of maxima and minima; $\Delta x = n\lambda$) is increased (constructive interference); while that of waves, in which the maxima of one coincide with the minima of the other, is reduced (destructive interference).



39. Continued.
Diffraction of x-ray is the result of scattering and interference in ordered structures (crystals). Coherent x-rays, scattered at atomic planes, will exhibit constructive interference in directions for which the scattered rays, at parallel planes, result in path differences of one or more λ . Coherent x-rays, scattered at parallel planes, will experience destructive interference in directions along which the scattered rays experience a path difference of $(n-1/2)\lambda$.
40. High quality Al single crystals will always have dislocations and “dislocation generators” which under stress generate more and more dislocations. Under stress, these dislocations move more readily in the slip system from one side of a crystal to the other; thus leading to slip, plastic deformation, limiting the tensile strength of aluminum. In fine grained Al you also have dislocations. In fact, there are many more than in the perfect crystal. When you apply stress, the dislocations move readily. However, they get arrested at the first grain boundary. Here stress may still persist and slip will be initiated, again along a slip plane, which no longer is in the same direction. The arrests of slip and changing slip directions from grain to grain lead to a significant reduction in the magnitude of deformation. The strength is increased.