1) 19.611, 28.136, 35.156, 41.546, 47.769, 54.119, 60.876, 69.212, 82.008

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

$\therefore$ ratio $\sin^2\theta$ = ratio $\underbrace{h^2+k^2+l^2}_{\text{give struct}}$

ration $\sin^2\theta$:

1 : 1.97 : 2.94 : 3.90 : 4.87 : 5.83 : 6.77 : 7.76 : 8.7

$\therefore$ bcc struct ✓

ii) $\lambda = 1.54 Å = 1.54 \times 10^{-10}$ m

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

$$\therefore \; a = \sqrt{\frac{\lambda^2}{4\sin^2\theta} \times (h^2+k^2+l^2)}$$

$\theta = 19.611 \;\; \therefore \; 110 \;\; 2 \;\; \Rightarrow a = \cancel{1.69} \times 10^{-10}$ m 3.244

$\theta = 28.136 \;\; \therefore \; 200 \;\; 4 \;\; \Rightarrow a = \cancel{1.53} \times 10^{-10}$ m 3.266

$\theta = 35.156 \;\; \therefore \; 211 \;\; 6 \;\; \Rightarrow a = 2.\cancel{95} \times 10^{-10}$ m 3.276

$\theta = 41.546 \;\; \therefore \; 220 \;\; 8 \;\; \Rightarrow a = 3.28 \times 10^{-10}$ m

3.28 ≠ 1.69

iii) $a = 3.\cancel{28} \times 10^{-10}$ m ✓
30

iv) lattice spacing = a?

spacing lattice plane cubic struct $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$

2) T = 293 K Bragg: 47.75°

T = 1273 K Bragg: 46.60°

$a(T') = a(T) \times [1 + \alpha(T' - T)]$

$\sqrt{\frac{\lambda^2}{4\sin^2\theta'} \times (h'^2+k'^2+l'^2)}$ … $\sqrt{\frac{\lambda^2}{\ldots} \times (h^2+k^2+l^2)}$

Coef lin expans $a, \alpha$?  $\sqrt{4 \sin^2\theta}$  $= \cancel{\sqrt{4 \sin^2\theta}}$

$\times \cancel{[1+\alpha(T'-T)]}$

$$a(T') = a(T) \times [1+\alpha(T'-T)]$$

Bragg's $n\lambda = 2d\sin\theta \quad \therefore d = \dfrac{n\lambda}{2\sin(\theta)}$

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

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

$$\therefore a = \sqrt{\frac{\lambda^2}{4\sin^2\theta} \times (h^2+k^2+l^2)}$$

$$\frac{a(T')}{a(T)} = 1 + \alpha(T'-T)$$

$$\frac{d_{1273}}{d_{293}} = \frac{\sin(47.75)}{\sin(46.6)} = 1.018$$

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}} \quad \therefore \quad \frac{d_{1273}}{d_{293}} = \frac{a_{1273}}{a_{293}} = 1 + \alpha(T'-T)$$

$$1.018 = 1 + \alpha(1273 - 293)$$

$$\frac{0.018}{980} = \alpha = 1.84 \times 10^{-5}\ K^{-1}$$

A4 or

So through logic!

3) CsCl

$E = 8.05$ keV

10.83° | 15.39° | 18.99° | 22.07° | 24.84°

i) $$a = \sqrt{\frac{\lambda^2}{4\sin^2\theta} \times (h^2+k^2+l^2)}$$

$$\lambda = \frac{hc}{E} = \frac{6.626 \times 10^{-34}\ Js \times 2.998 \times 10^{8}\ m/s}{8.05 \times 10^3 \times 1.602 \times 10^{-19}\ J}$$

$= 1.54 \times 10^{-10}$ $\cancel{Js}$ m/s $\cancel{J^{-1}}$ ✓

$= 1.54$ Å

$$a_{10.83} = \frac{2.37 \times \cancel{10^{-20}}\ \cancel{(2)}}{4 \sin^2(10.83)} \approx \cancel{3.39}\ Å$$

2

~~5.8~~

~~5.8~~

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

CsCl ~ bcc

$$a_{18.99} = \frac{2.37 \times \cancel{10^{-20}}}{4\sin^2(18.99)} \times 6 \approx \cancel{3.36}\ Å$$

ii) ~~110~~

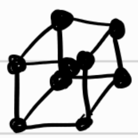
~~200~~
~~211~~
~~220~~ nope

4) i) ice – H $Z=1$, O $Z=8$  Neutron  H invisible xrays
ii) MgO – Mg $Z=12$, O $Z=8$  Xrays
iii) U – elemental solid  Xrays
iv) AgO – $Z$ 47, $Z$ 8  Neutron

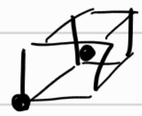
5) Laue condit's – must be satisfied for diffrat° to occur
$$\begin{cases} \vec{Q}\cdot\vec{a} = 2\pi h \\ \vec{Q}\cdot\vec{b} = 2\pi k \\ \vec{Q}\cdot\vec{c} = 2\pi l \end{cases}$$

Struct factor – influences relative intensities of diffrac° spots / lines
$$S(\vec{Q}) = \sum_{\nu} f_{\nu} e^{-i\vec{Q}\cdot\vec{r}_{\nu}}$$
$$= \sum_{\nu} f_{\nu} e^{-2\pi i(hu+kv+lw)}$$

i) bcc



2 atom basis

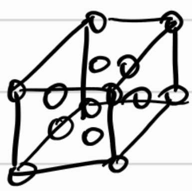


$(u,v,w) = (0,0,0), (\frac{1}{2},\frac{1}{2},\frac{1}{2})$

$$S(\vec{Q}) = \sum_{\nu} f_{\nu} e^{-2\pi}$$

$$\begin{aligned} S^{\text{bcc}}_{hk\ell} &= \sum_{\mu=1}^{2} f_{\mu} e^{-2\pi i(hu+kv+\ell w)} \\ &= f \times \left(1 + e^{-i(h+k+\ell)\pi}\right) \\ &= f \times \left(1 + (-1)^{h+k+\ell}\right) = \begin{cases} f \times 2 & h+k+\ell \text{ even} \\ f \times 0 & h+k+\ell \text{ odd} \end{cases} \end{aligned}$$

ii) fcc



4 atom basis  $(u,v,w) = (0,0,0), (\frac{1}{2},\frac{1}{2},0), (\frac{1}{2},0,\frac{1}{2}), (0,\frac{1}{2},\frac{1}{2})$

$$S^{fcc}_{hkl} = \sum_{\mu=1}^{4} f_{\mu} e^{-2\pi i(hu+kv+lw)}$$
$$= f \times \left(1 + e^{-i(h+k)\pi} + e^{-i(h+l)\pi} + e^{-i(k+l)\pi}\right)$$
$$= f \times \left(1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right)$$

ODD → / EVEN ↓

| | h | k | l |
|---|---|---|---|

E / ODD → / E / ODD ↓

| | h | k | l |
|---|---|---|---|

| | | | |
|---|---|---|---|
| h | × | -1 | -1 |
| k | -1 | × | -1 |
| l | -1 | -1 | × |

| | | | |
|---|---|---|---|
| h | × | 1 | 1 |
| k | 1 | × | 1 |
| l | 1 | 1 | × |

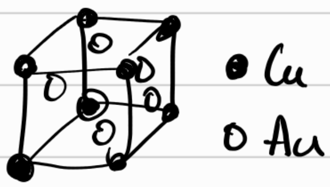
$$= \begin{cases} f \times 4 & h, k, l \text{ all odd or even} \\ f \times 0 & \text{otherwise} \end{cases}$$

iii) sc

$$(u,v,w) = \underbrace{(0,0,0)}_{Cu} \quad \overbrace{(\tfrac{1}{2}, \tfrac{1}{2}, 0) \quad (\tfrac{1}{2}, 0, \tfrac{1}{2}) \quad (0, \tfrac{1}{2}, \tfrac{1}{2})}^{Au}$$

$$S(\vec{Q}) = \sum_{\nu} f_{\nu} e^{-2\pi i (hu + kv + lw)}$$

↑ diff for diff atoms




$$\cancel{= f \times \left(1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right)}$$

$$\cancel{= \begin{cases} f \times 4 & \text{all odd/even} \\ f \times 0 & \text{otherwise} \end{cases}}$$

$$= f_{Cu} + f_{Au}\left((-1)^{h+k} + (-1)^{h+l} + (-1)^{kl}\right)$$

$$= \begin{cases} f_{Cu} + 3_{Au} & \text{if } h, k, l \text{ all odd/even} \\ f_{Cu} & \text{otherwise} \end{cases}$$

6) i) fcc $\quad a = 4.05$ Å $\quad z = 3$

↓

4 atom basis $\quad N = 4$

$V = a^3 = 66.43$ Å$^3$

$$n = z \frac{N}{V} = \frac{3 \times 4}{66.43} \approx 0.18 \text{ Å}^{-3}$$

ii) bcc $\quad z = 1$

↓ mass density $10^3$ kg/m$^3$

2at  atomic weight 23 amu = $3.818 \times 10^{-26}$ kg

$$\text{mass density} = \frac{\text{mass}}{\text{vol}} = \text{n° atoms} \times \text{atomic weight}$$

$$\text{vol} = \frac{2\times 3.818 \times 10^{-26}}{10^{3}} = 2\times 3.818 \times 10^{-29}\ m^{3}$$

$$n = Z\frac{N}{V} = \frac{2}{3.818\times10^{-29}} = 5.24\times10^{28}$$

7) $\sigma = \frac{ne^2\tau}{m}$  $\rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau}$  $m = 9.1\times10^{-31}$  $e = 1.6\times10^{-19}$

$\tau = \frac{\sigma m}{ne^2}$

| Element | resistivity $\rho$ ($\mu\Omega$-cm) | conductivity $\sigma$ ($10^6$ S cm$^{-1}$) | scattering time $\tau$ ($10^{-14}$ secs) |
|---|---|---|---|
| Na (77 K) | 0.8 | 1.25 | 17 |
| Ag (273 K) | 1.51 ✓ | 0.66 | ~~2.34~~ 4 |
| Mg (273 K) | 3.2~~3~~9 | 0.3~~1~~26 | 1.1 |
| Al (373 K) | 3.55 | 0.28 ✓ | ~~0.99~~ 0.55 |

redo Mg

redo $\tau$

$C = \frac{V}{\Omega}$

Mg  $\tau = 1.1$  ~~$\sigma = \frac{ne^2 T}{m} = 3.09\times10^{-22}\ C.s.kg^{-1} = 3.09\times10^{-22}\ \frac{V}{\Omega} s\ kg^{-1}$~~

$n = 1$

$m = 9.1\times10^{-31}$ kg

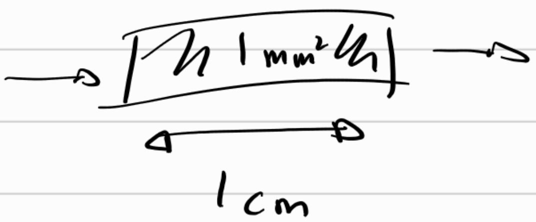
$e = 1.6\times10^{-19}$ C

$\tau = 1.1\times10^{-14}$ s

$$\rho = \frac{m}{ne^2\tau} = \frac{9.1\times10^{-31}}{1\times1.6\times10^{-19}\times1.1\times10^{-14}} = 517.04$$

$\mu\Omega$ cm  kg $C^{-1} s^{-1}$

8)




~~$R = 2\times10^{-4}\ \Omega$~~

~~$\rho = 2\times10^{-?}\ \Omega$~~

resistance

$R = \rho L$  $\rho = \frac{m}{ne^2\tau}$  $R = 2\times10^{-4}\ \Omega$

resistivity $A$ $\tau = \dfrac{m}{ne^2 \rho}$

$\rho = \dfrac{RA}{L} = \dfrac{2\times10^{-4} \times 10^{-1}\ \Omega\, cm^2}{1\ \cancel{cm}}$

$= 2\times10^{-5}\ \Omega\, cm$

$\tau = \dfrac{m}{ne^2\rho}$ kg, s, $\Omega cm$, $C^2$

$n = 5.9\times10^{22}\ cm^{-3} = 5.9\times10^{28}\ m^{-3}$ notes

$m = 9.1\times10^{-31}$ kg, $e = 1.6\times10^{-19}$ C given

how does this relationship work

$\tau = \dfrac{9.1\times10^{-31}\ \Omega\, cm}{5.9\times10^{22}\times(1.6\times10^{-19})^2\times 2\times10^{-5}}$ $cm^{-2}$ kg C

$= 3.01\times10^{-11}\ cm^3\ \Omega\ kg^{-1} C^{-1}$

units problem

Continue in ex 9 ~ see past ex tutorial

9) $\dfrac{d\vec{p}}{dt} = \vec{F} - \dfrac{\vec{p}}{\tau}$

steady state current flows with current density : $\vec{j} = \sigma\vec{\varepsilon}$ , $\sigma$?

Steady state $\dfrac{d}{dt} \to 0$ $\therefore$ $\dfrac{d\vec{p}}{dt} = F - \dfrac{p}{\tau} = 0$

$-e\varepsilon - \dfrac{\vec{p}}{\tau} = 0$

$\vec{p} = -e\tau\varepsilon$

electrons average velocity $\vec{v} = \dfrac{\vec{p}}{m} = -\dfrac{e\tau}{m}\varepsilon$

current density : $n\cdot e\cdot\vec{v} = \dfrac{ne^2\tau}{m}\varepsilon$

$\sigma = \dfrac{ne^2\tau}{m}$

$2.7\times10^{-8} = \sigma^{-1} = \dfrac{m}{ne^2\tau}$

$\tau = \dfrac{m}{ne^2\rho} = 0.73\times10^{-14}$ sec

$n = 18\times10^{22}\ cm^{-3}$

$m = 9.1\times10^{-31}$

10) $\tau \propto \rho \to T$?

$\rho = \dfrac{m}{ne^2\tau}$

mean free path $l = v\tau$ $\therefore$ $v = \dfrac{l}{\tau}$

Drude $\frac{1}{2}m\langle v\rangle^2 = \frac{3}{2}k_B T$

$\therefore \frac{1}{2}m\frac{l}{\ldots} \quad \frac{3}{2}k_B T$

tutorial

$$\frac{m l}{3 k_B} \frac{1}{\tau} = T \quad \Leftarrow \text{linear relation}$$

$$l = \frac{T \tau 3 k_B}{m}$$

ii) 

when $B$ is applied electrons move in opposite direc° to classical current $\vec{j}$ ∴ Lorentz force bends trajectories

→ $E$ cannot pass through the edge, leading to net accumulat° of negative charge

next ?