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HW#2 solutions

Physics 406

(1.) O. Ch. 2, Q. 1

The scattered rays are nearly parallel because the detector is far away from the crystal, so the plane-wave approximation is valid.

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(2.) O. Ch. 2, Q. 5

The lattice structure factors will be the same since they are both fcc. However, the diffraction patterns will have different spacings reflecting different unit cell dimensions.

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(3.) O. Ch. 2, Q. 7

No, there is no one-to-one correspondence. Reciprocal lattice vectors are normal to a set of crystal planes, which are defined by two direct lattice vectors.

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(4.) O Ch. 2, Q. 9

For crystal diffraction we need $\lambda = O(1)\,\text{Å}$ ~ interatomic spacing

Let's define $\lambda_0 = 1\,\text{Å}$.

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Using de Broglie relations,

$$\lambda_0 = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \Rightarrow \text{Need } E = \frac{h^2}{2m\lambda_0^2}.$$

Since $m_n > m_{\bar{e}}$ & $E \sim \frac{1}{m}$, $E_n < E_{\bar{e}}$.

(n ← neutron, $\bar{e}$ ← electron)

5. O. Ch. 2, Pr. 1

Recall that

$$\lambda_{min} = \frac{12.3}{V(kV)}\ \text{Å}\ ;$$

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$$V(kV) = \frac{12.3}{1.23} = \underbrace{10^4\ V}_{10\ kV}.$$

The kinetic energy

$$KE = eV = 10^4\ \underline{\underline{eV}}.$$

⑥ Ch. 2, Pr. 2

proven in another problem

Using $d_{hkl} = \frac{2\pi}{G_{hkl}}$ & the fact that the reciprocal of a cubic lattice is a cubic lattice, we obtain: $G_{hkl} = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2}$,

which gives

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

With $a = 2.62$ Å,

$d_{100} = a = 2.62$ Å, $d_{110} = \frac{a}{\sqrt{2}} = 1.85$ Å,

$d_{111} = \frac{a}{\sqrt{3}} = 1.51$ Å, $d_{200} = \frac{a}{2} = 1.31$ Å,

5|5 $d_{210} = \frac{a}{\sqrt{5}} = 1.17$ Å, $d_{211} = \frac{a}{\sqrt{6}} = 1.07$ Å.

Then the 1st order Bragg reflection gives $\sin\theta_{hkl} = \frac{\lambda}{2d_{hkl}}$.

With $\lambda = 1.54$ Å,

$\sin\theta_{100} = 0.294 \Rightarrow \theta_{100} = 17.1°$

Likewise, $\begin{cases} \theta_{110} = 24.6°, & \theta_{210} = 41.1°; \\ \theta_{111} = 30.6°, & \theta_{211} = 46.0°. \\ \theta_{200} = 36.0°, & \end{cases}$

Note that smaller interplanar distances correspond to larger angles.

7. θ. Ch. 2, Pr. 3

a) $\lambda = 1.54$ Å

$\theta = 19.2°$ (111) planes

Bragg's law: $n\lambda = 2d\sin\theta$.

5/5 assuming $n=1$,

$$d_{111} = \frac{\lambda}{2\sin\theta} = \frac{1.54\text{ Å}}{2\cdot\sin(19.2°)} \approx 2.34\text{ Å}$$

b)

$$\rho = \frac{\#\text{ Al atoms}}{\text{unit cell volume}} \times \frac{\text{mol. weight of Al}}{N(\#\text{ atoms in 1 mole})}$$

Al is fcc: $8\times\frac{1}{8} + 6\times\frac{1}{2} = 4 \frac{\text{atoms}}{\text{unit cell}}$.

$V = a^3$ unit cell volume

(8.) The plane $(hk\ell)$ is defined by its intercepts

$$\frac{\vec{a}_1}{h}, \quad \frac{\vec{a}_2}{k}, \quad \frac{\vec{a}_3}{\ell}$$

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(a) Define $\begin{cases} \vec{A} = \dfrac{\vec{a}_1}{h} - \dfrac{\vec{a}_2}{k}, \\ \vec{B} = \dfrac{\vec{a}_1}{h} - \dfrac{\vec{a}_3}{\ell} \end{cases}$

These 2 vectors are in the plane.

$$\vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3 =$$

$$= \frac{2\pi}{V} h(\vec{a}_2 \times \vec{a}_3) + \frac{2\pi}{v} k(\vec{a}_3 \times \vec{a}_1) +$$

$$+ \frac{2\pi}{V} \ell(\vec{a}_1 \times \vec{a}_2)$$, where V is the unit cell volume.

Then $\vec{G} \cdot \vec{A} = 2\pi - 2\pi = 0$,

$\vec{G} \cdot \vec{B} = 0$.

$\vec{G}$ is $\perp$ to $(hk\ell)$.

(b) Let $\hat{n}$ be the unit normal to the plane $(hk\ell)$.

$\frac{\vec{a}_1}{h} \cdot \hat{n} = d_{hk\ell}$ (projection of $\frac{\vec{a}_1}{h}$ onto $\hat{n}$)

But $\hat{n} = \frac{\vec{G}}{|\vec{G}|}$, as shown in (a).

Then $d_{hkl} = \frac{\vec{a}_1 \cdot \vec{G}}{h|\vec{G}|} = \frac{2\pi}{|\vec{G}|}$.

(c) For an sc lattice,

$$\vec{G} = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z})$$

$$d^2_{hkl} = \frac{4\pi^2}{G^2} = \frac{4\pi^2}{\left(\frac{2\pi}{a}\right)^2 (h^2+k^2+l^2)} =$$

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

(9) Key points of Handout 3:

(a) Oblate spheroids pack more densely than do spheres when poured randomly & shaken.

(b) More experiments with different spheroid aspect ratios & computer simulations show that random packing densities can approach the perfect

5/5 packing ratio of 0.74.

(c) It was always assumed that periodic orderings are denser than random ones ⇒ true for spheres but may not be true for all spheroids.

(d) Changes in spheroid shape may lead to major changes in random packing densities.