35/35 HW #2 solutions | Physics 406

(1.) Θ. Ch. 2, Q. 1

2/2 The scattered rays are nearly parallel because the detector is located very far away from the crystal.

(2.) Θ Ch. 2, Q. 5

3/3 The lattice structure factor will be the same since they are both fcc. The atomic form factors will be different however.

(3.) Θ Ch. 2, Q. 10

acc. to Bragg's law,

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

5/5 and so there is no diffraction for $\lambda > 2d$ (since $\sin\theta \leq 1$). Roughly, we need $\lambda \sim d$.

ie $\lambda = 5100\,\text{Å}$ (visible green light), $d \simeq 5000\,\text{Å}$, 10^3 times greater than what we see in nature.

4. O. Ch. 2, Pr. 1

Recall that

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

5/5

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

The kinetic energy

$$KE = eV = 10^4 eV.$$

5. O. 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 $n=1$,

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

b)

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

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

For fcc lattice

$$d = \frac{a}{\sqrt{h^2+k^2+\ell^2}}, \text{ or}$$

$$a = d_{111}\sqrt{3} \simeq 4.05 \text{ Å}$$

So, $$N = \frac{\# \text{ Al atoms}}{V} \times \frac{M(\text{Al})}{\rho} =$$

$$= \frac{4}{(4.05 \times 10^{-8})^3 \text{ cm}^3} \times \frac{27 \text{ g/mole}}{2.7 \text{ g/cm}^3} =$$

$$= \frac{4}{(4.05)^3} \times 10^{25} \text{ atoms/mole} \simeq$$

$$\simeq 6.02 \times 10^{23} \text{ atoms/mole.}$$

Avogadro's number

(6.) 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,

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

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

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

(7.) By definition,

$$\vec{b}_1 = 2\pi \left(\frac{a}{2}\right)^2 \frac{(\hat{z}+\hat{x})\times(\hat{x}+\hat{y})}{V},$$

5|5 where $V = \left(\frac{a}{2}\right)^3 (\hat{y}+\hat{z})\cdot[(\hat{z}+\hat{x})\times(\hat{x}+\hat{y})] =$

$$= \left(\frac{a}{2}\right)^3 (\hat{y}+\hat{z})\cdot(\hat{y}-\hat{x}+\hat{z}) =$$

$$= 2\left(\frac{a}{2}\right)^3.$$

So, $\vec{b}_1 = \frac{2\pi (a/2)^2}{2(a/2)^3}(\hat{y}-\hat{x}+\hat{z}) =$

$$= \frac{2\pi}{a}(\hat{y}-\hat{x}+\hat{z}).$$

Likewise,

$$\vec{b}_2 = \frac{2\pi}{a}(\hat{x}+\hat{y})\times(\hat{y}+\hat{z}) =$$

$$= \frac{2\pi}{a}(\hat{z}-\hat{y}+\hat{x}),$$

$$\vec{b}_3 = \frac{2\pi}{a}(\hat{y}+\hat{z})\times(\hat{z}+\hat{x}) =$$

$$= \frac{2\pi}{a}(\hat{x}-\hat{z}+\hat{y})$$

This is a bcc lattice, the lattice const is $\frac{4\pi}{a}$.

(8.) It is known that the packing ratio of spheres into an fcc lattice is $\varphi \simeq 0.74$. ~~However~~, $\varphi \simeq 0.64$ for random jammed packings (amorphous solids). Here the authors show, by experiments and computer simulations, that φ up to 0.74 can be achieved using ellipsoids. This dense packing is accompanied by an increased number of contacts per particle, up to 10 for ellipsoids vs. 6 for spheres.

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