UNOFFICIAL SOLUTIONS BY TheLongCat

B3: VI. CONDENSED-MATTER PHYSICS

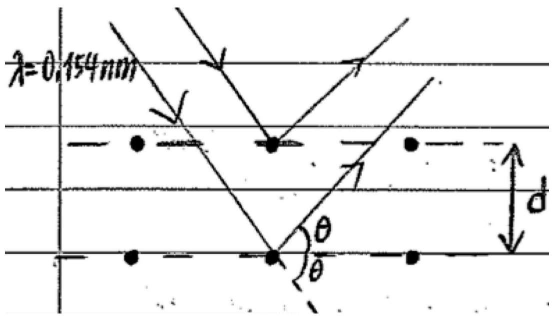
TRINITY TERM 2012

Last updated: 30th May 2025

Turn over as you please – we are NOT under exam conditions here.

1. **(DRAFT)**

(a) For EM wave to interact with a nucleus, it must possess wavelength of $\sim$ fm range, this corresponds to gamma rays and therefore X-rays do not interact with it well. X-rays are therefore only affected by the bound e^- in an atom.



Bragg's Law:

$$2d\sin\theta = \lambda$$
$$\Rightarrow d = \frac{\lambda}{2\sin\theta}$$

Total diffraction angle: 2θ

For cubic lattice,

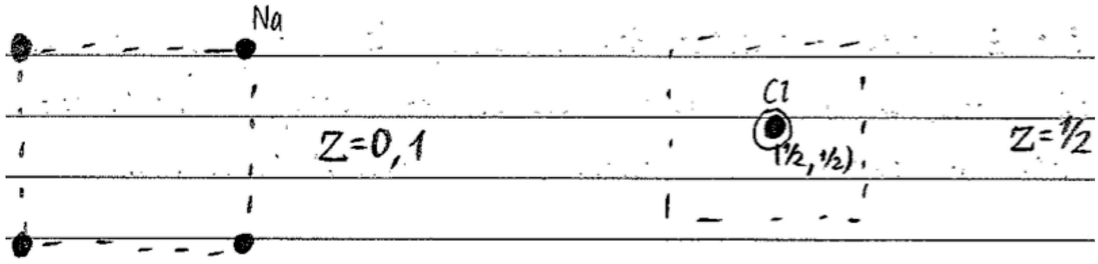
$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$
$$\Rightarrow h^2+k^2+l^2 = \left(\frac{a}{d}\right)^2$$

2θ (°)	d (nm)	$\frac{d_0}{d} \to \left(\frac{d_0}{d}\right)^2$	$h^2+k^2+l^2$	a (nm)
27.4	$0.325 = d_0$	$1 \to 1$	$3 = 1^2+1^2+1^2$	0.563
31.7	0.282	$1.15 \to 1.33$	$4 = 2^2+0^2+0^2$	0.564
45.4	0.200	$1.63 \to 2.65$	$8 = 2^2+2^2+0^2$	0.566
53.8	0.170	$1.91 \to 3.65$	$11 = 3^2+1^2+1^2$	0.564

Since h, k, l all have the same parity, NaCl is an FCC crystal in this condition.

Lattice constant:

$$\begin{aligned} a &= \sqrt{h^2+k^2+l^2}d \\ &= \frac{1}{4}(0.563+0.564+0.566+0.564) \\ &= 0.564\,(\text{nm}) \end{aligned}$$



(b) Scattering amplitude now becomes:

$$S_{(hkl)} = f_{\mathrm{Na}} + f_{\mathrm{Cl}} e^{i\pi(h+k+l)}$$

Since $f_{\mathrm{Na}} \neq f_{\mathrm{Cl}}$, and the fact that NaCl is now a simple cubic lattice means that any h, k, l constitute a diffraction peak.

Minimum diffraction angle should then correlates to the $\{100\}$ family:

$$a = d_0 = \frac{\lambda}{2\sin\theta} = 0.300\,\mathrm{nm}$$

Next ring should be due to the $\{110\}$ family:

$$\begin{aligned} d_{\{110\}} &= \frac{a}{\sqrt{1^2+1^2+0^2}} = 0.212\,\mathrm{nm} \\ \Rightarrow \sin\frac{1}{2}\theta_{\{110\}} &= \frac{\lambda}{2d_{\{110\}}} \\ &= 0.362 \\ \Rightarrow \theta_{\{110\}} &= 42.5^\circ \end{aligned}$$

Ratio of intensity:

$$\frac{I_{\{110\}}}{I_{\{100\}}} = \frac{M_{\{110\}}}{M_{\{100\}}} \left|\frac{S_{\{110\}}}{S_{\{100\}}}\right|^2$$

where $M_{\{110\}} = 12$ and $M_{\{100\}} = 6$ are multiplicities associated with the corresponding family.

Since $f_i \propto Z_i$ for atom i, we write:

$$f_{\mathrm{Na}} = 11f \qquad f_{\mathrm{Cl}} = 17f$$

with constant of proportionality f.

Structure factors read:

$$\begin{aligned} S_{\{110\}} &= 11f + 17fe^{i2\pi} = 28f \\ S_{\{100\}} &= 11f + 17fe^{i\pi} = -6f \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{I_{\{110\}}}{I_{\{100\}}} &= \frac{12}{6}\left|\frac{28}{-6}\right|^2 \\ &= 43.56 \end{aligned}$$

$$\begin{aligned}\text{Ratio of volume} &= \left(\frac{a_{80\,\mathrm{GPa}}}{a_{\mathrm{STP}}}\right)^3 \\ &= \left(\frac{0.300}{0.564}\right)^3 = 0.150\end{aligned}$$

2. (DRAFT)

(a) Debye model:

- Atoms behave like a harmonic oscillator independent to its immediate neighbours.
- The oscillation is quantised such that the quantisation (phonons) obeys the Bose-Einstein statistics.
- Linear phonon dispersion $\omega = vk$.

von Karman boundary condition:

$$\sum_{\mathbf{k}} \to \frac{V}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k}$$

Total energy:

$$\begin{aligned} E &= 3 \cdot \frac{V}{(2\pi)^3} \int_0^\infty 4\pi k^2 \cdot \hbar\omega \cdot \left(n_\mathrm{B} + \frac{1}{2} \right) \mathrm{d}k \quad \text{where } n_\mathrm{B} = \frac{1}{e^{\beta\hbar\omega} - 1} \\ &= \frac{3V}{2\pi} \int_0^\infty \frac{1}{v} \left(\frac{\omega}{v} \right)^2 \hbar\omega \cdot \frac{1}{e^{\beta\hbar\omega} - 1} \, \mathrm{d}\omega \end{aligned}$$

Make substitution $x = \beta\hbar\omega \Rightarrow \mathrm{d}x = \beta\hbar \, \mathrm{d}\omega$:

$$\begin{aligned} \Rightarrow E &= \frac{3V}{2\pi} \int_0^\infty \frac{1}{\beta\hbar v} \frac{\hbar}{v^2} \cdot \left(\frac{x}{\beta\hbar} \right)^3 \cdot \frac{1}{e^x - 1} \, \mathrm{d}x \\ &= \frac{3V}{2\pi} \cdot \frac{1}{\beta^4 v^3 \hbar^3} \int_0^\infty \frac{x^3}{e^x - 1} \, \mathrm{d}x \end{aligned}$$

Hence heat capacity:

$$\begin{aligned} C &= \frac{\partial E}{\partial T} \\ &= \frac{6V k_\mathrm{B}^4 T^3}{v^3 \hbar^3} \int_0^\infty \frac{x^3}{e^x - 1} \, \mathrm{d}x \end{aligned}$$