

$$1. (a) \text{ no. of Si atoms per unit cell} = \frac{1}{8} \times 8 + \frac{1}{2} \times 6 + 4 \\ = 8$$

$$(b) \text{ No. of Ca atoms per unit cell} = 4$$

$$\text{No. of As atoms per unit cell} = \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$$

$$(c) \rho = \frac{\text{Total mass of atoms in a unit cell}}{a^3}$$

$$= \frac{4(m_{\text{Ga}} + m_{\text{As}})}{a^3}$$

$$\Rightarrow a = \left(\frac{4(m_{\text{Ga}} + m_{\text{As}})}{\rho} \right)^{\frac{1}{3}} = \left(\frac{4(\text{molar mass of Ga} + \text{molar mass of As})}{N_A \rho} \right)^{\frac{1}{3}}$$

$$= \left(\frac{4(69.723 + 74.923) \text{ g mol}^{-1}}{(6.022 \times 10^{23} \text{ mol}^{-1})(5.3176 \times 10^6 \text{ g m}^{-3})} \right)^{\frac{1}{3}} \quad \begin{array}{l} N_A \rho \\ \text{no. of particles} \\ \text{per mole.} \end{array}$$

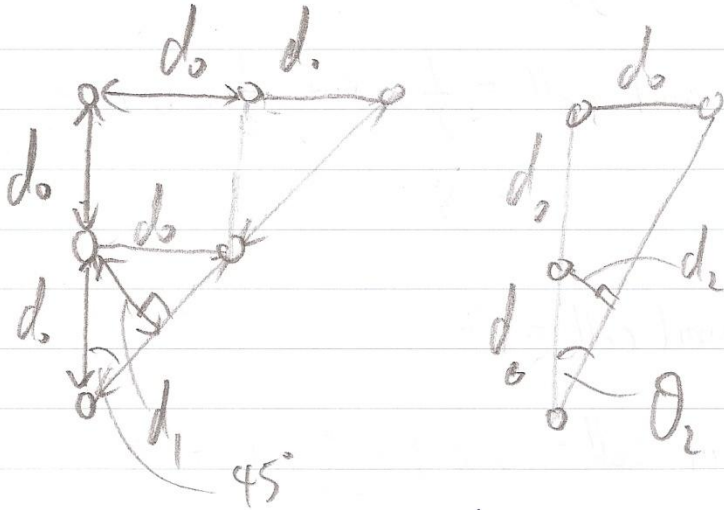
$$= 5.65 \times 10^{-10} \text{ m}$$

$$= 5.65 \text{ \AA}$$

Alternatively, if we take $m_{\text{Ga}} = 69.723 \text{ u}$, $m_{\text{As}} = 74.923 \text{ u}$, where $u = 1.66 \times 10^{-27} \text{ kg}$

$$\text{Then } a = \left(\frac{4(69.723 + 74.923) \text{ u}}{(5.3176 \times 10^6 \times 10^{-3}) \text{ kg m}^{-3}} \right)^{\frac{1}{3}} = 5.65 \text{ \AA}$$

2. (a)



$$d_1 = d_0 \sin 45^\circ = \frac{d_0}{\sqrt{2}}$$

$$\sin \theta_2 = \frac{1}{\sqrt{5}}$$

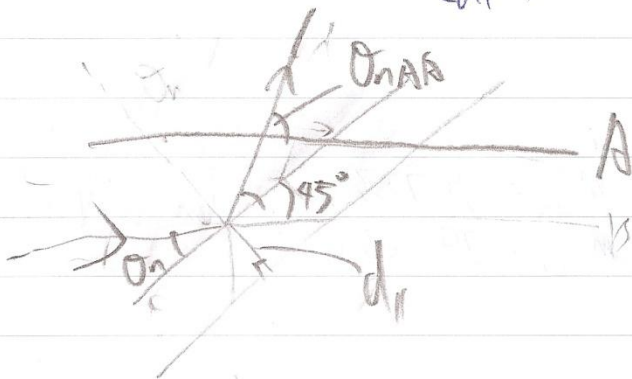
$$\therefore d_2 = d_0 \sin \theta_2 = \frac{d_0}{\sqrt{5}}$$

$$(b) \quad 2d_1 \sin \theta_n = n\lambda, \quad d_1 = \frac{4}{\sqrt{2}} = 2.83 \text{ \AA}, \quad \lambda = 0.626 \text{ \AA}$$

$$\Rightarrow \theta_1 = \sin^{-1} \left(\frac{\lambda}{2d_1} \right) = \sin^{-1} \left(\frac{0.626}{2(2.83)} \right) = 6.5^\circ$$

$$\theta_2 = \sin^{-1} \left(\frac{2\lambda}{2d_1} \right) = \sin^{-1} \left(\frac{0.626}{2.83} \right) = 12.8^\circ$$

$$\theta_3 = \sin^{-1} \left(\frac{3\lambda}{2d_1} \right) = \sin^{-1} \left(3 \cdot \frac{0.626}{2(2.83)} \right) = 19.4^\circ$$



$$\theta_{nAA} = \theta_n + 45^\circ$$

$$\Rightarrow \theta_{1AA} = 51.5^\circ$$

$$\theta_{2AA} = 57.8^\circ$$

$$\theta_{3AA} = 64.4^\circ$$

$$3. (a) eV_A = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$$

$$\Rightarrow \lambda = \frac{h}{\sqrt{2meV_A}}$$

$$(b) 2d \sin \theta = \lambda$$

For small θ , $\sin \theta \approx \theta$

$$\text{where } 2\theta \approx \frac{D}{2L},$$

$$\text{and } \lambda = \frac{h}{\sqrt{2meV_A}},$$

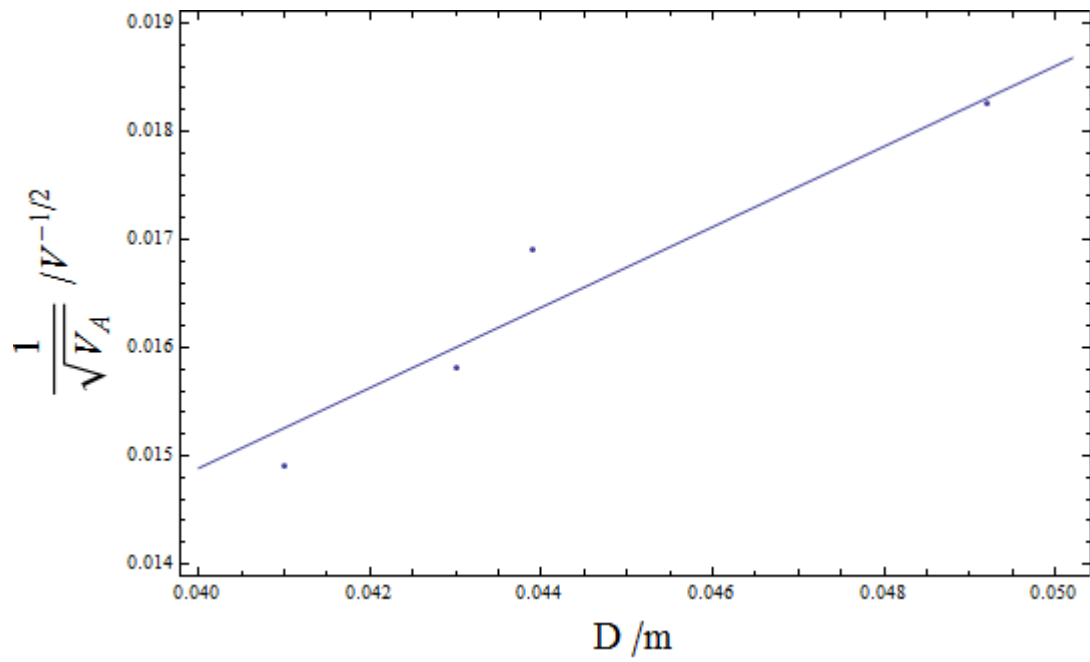
$$\therefore 2d \sin \theta \approx \frac{Dd}{2L} = \frac{h}{\sqrt{2meV_A}}$$

$$\Rightarrow D = \frac{2hL}{d\sqrt{2me}} \frac{1}{\sqrt{V_A}} \Rightarrow \frac{1}{\sqrt{V_A}} = \frac{d\sqrt{2me}}{2hL} D$$

(c) Slope of the curve of $\frac{1}{\sqrt{V_A}}$ v.s. D is $= 0.372 \text{ V}^{-\frac{1}{2}} \text{ m}^{-1}$

$$\therefore 0.372 = \frac{d\sqrt{2me}}{2hL} = \frac{d \sqrt{(9.11 \times 10^{-31})(1.6 \times 10^{-19})}}{\sqrt{2}(6.63 \times 10^{-34})(0.130)}$$

$$\Rightarrow d = 1.19 \text{ \AA}$$



The line is the best fit line: $y = 0.372 x$,
where $y = 1/\text{sqrt}[V_A]$, $x = D$.

Note that the fitted curve should pass through the origin.