

Diamantstruktur

a) $d = \frac{\sqrt{2}a}{4}$

$$\theta = 2 \arctan\left(\frac{4d}{a}\right) = 2 \arctan(\sqrt{2}) = \underline{\underline{109.47^\circ}}$$

b) $V = a^3; \quad r_{\text{fcc}} = \frac{a}{2\sqrt{2}}; \quad r_{\text{dia}} = \frac{a\sqrt{3}}{8}$

$$V_{\text{fcc}} = \frac{16}{3} \pi r_{\text{fcc}}^3 = \frac{\pi a^3}{3\sqrt{2}}$$

$$\frac{V_{\text{fcc}}}{V} = \frac{\pi}{3\sqrt{2}} \approx \underline{\underline{74\%}}$$

$$V_{\text{dia}} = 8 \frac{4}{3} \pi r_{\text{dia}}^3 = \frac{\sqrt{3}\pi a^3}{16}$$

$$\frac{V_{\text{dia}}}{V} = \frac{\sqrt{3}\pi}{16} \approx \underline{\underline{34\%}}$$

c) $\text{APF}_{\text{bcc}} \approx 68\%; \quad \text{APF}_{\text{sc}} \approx 52\%; \quad \text{APF}_{\text{hcp}} \approx 74\%$

Diamonds form by quite a margin the least dense crystal

d) $\rho = 3.51 \text{ g/cm}^3$

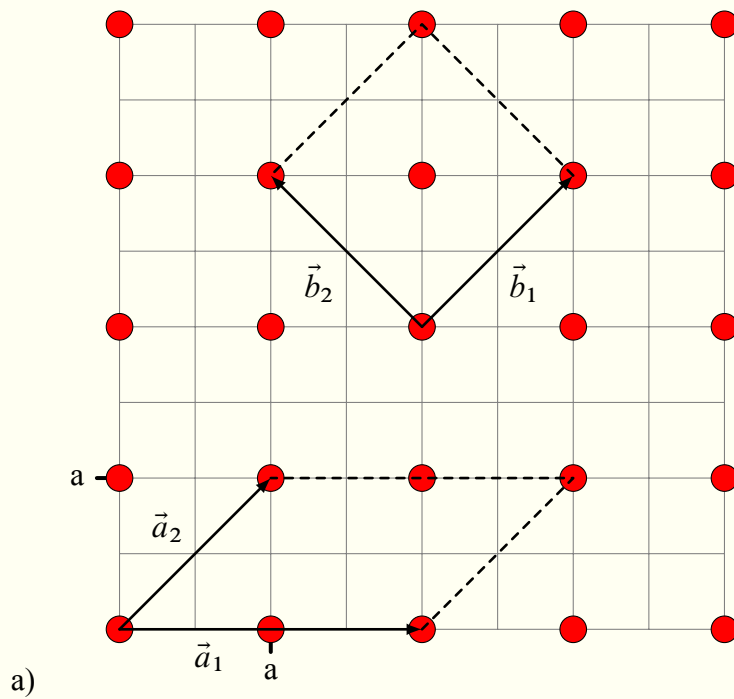
$$8m_{\text{C}} = \rho V_{\text{dia}}$$

$$r_{\text{dia}}^3 = \frac{3m_{\text{C}}}{\rho\pi 4}$$

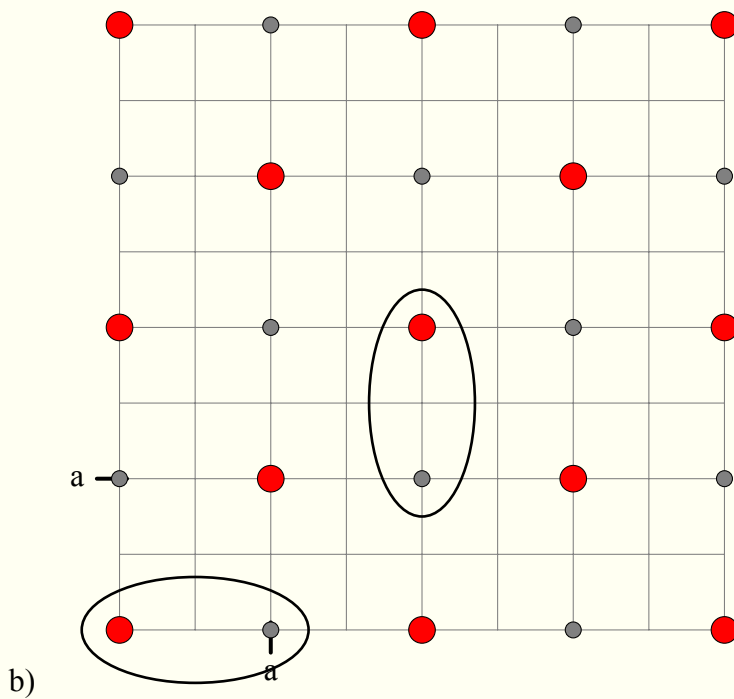
$$r_{\text{dia}} = \underline{\underline{1.11 \times 10^{-10} \text{ m}}}$$

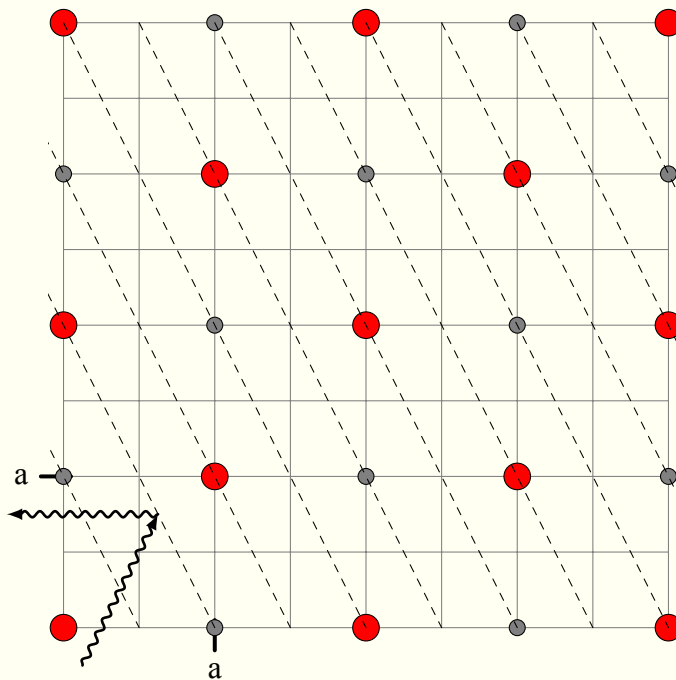
Gitter, Kristallstruktur und Röntgenbeugung

$$\vec{a}_1 = 2a\vec{e}_x; \quad \vec{a}_2 = a(\vec{e}_x + \vec{e}_y); \quad \vec{a}_3 = a\vec{e}_z; \quad \vec{r}_{\text{A}} = 0; \quad \vec{r}_{\text{B}} = \vec{a}_1/2$$



The unit cell is not primitive, as it contains more than one lattice point





c)

The X-Ray gets reflected by the crystal and leaves in the negative x-Direction

d) $\lambda = 1.46 \text{ \AA}$; $\theta = 15^\circ$

$$2a \sin(\theta) = n\lambda$$

$$a = \frac{\lambda}{2 \sin(\theta)} = \underline{\underline{2.82 \text{ \AA}}}$$

e) $\{h, k, l\} = (210)$; $\{u_1, v_1, w_1\} = (0, 0, 0)$; $\{u_2, v_2, w_2\} = (0.5, 0, 0)$

$$F_{210} = f_A + f_B e^{2i\pi} = \underline{\underline{f_A + f_B}}$$

Kristallstruktur von BaTiO₃

$$\text{a) } \vec{r}_1 = a \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \quad \vec{r}_2 = a \begin{pmatrix} 0.5 \\ 0.5 \\ 0 \end{pmatrix}; \quad \vec{r}_3 = a \begin{pmatrix} 0 \\ 0.5 \\ 0.5 \end{pmatrix}; \quad \vec{r}_4 = a \begin{pmatrix} 0.5 \\ 0 \\ 0.5 \end{pmatrix}; \quad \vec{r}_5 = a \begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \end{pmatrix}$$

The resulting bravais lattice is a simple cubic (sc) lattice.

b) $f_{\text{Ba}} : f_{\text{Ti}} : f_{\text{O}} = 3f_0 : 2f_0 : f_0; \quad \{h, k, l\} = (110)$

$$\begin{aligned} F_{110} &= f_{\text{Ba}} + f_{\text{Ti}} e^{2i\pi} + f_{\text{O}} e^{2i\pi} + 2f_{\text{O}} e^{i\pi} = \\ &= 3f_0 + 2f_0 + f_0 - 2f_0 = \underline{\underline{4f_0}} \end{aligned}$$

c) $a_0 = 0.4 \text{ nm}; \quad \lambda_R = 0.25 \text{ nm}$

$$d = \frac{a_0}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{a_0}{\sqrt{3}}$$

$$\lambda_R = 2d \sin(\theta)$$

$$\theta = \arcsin\left(\frac{\lambda_R \sqrt{3}}{2a_0}\right) = \underline{\underline{32.77^\circ}}$$