Alexander Helbok

Blatt 11

Diamantstruktur

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

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

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

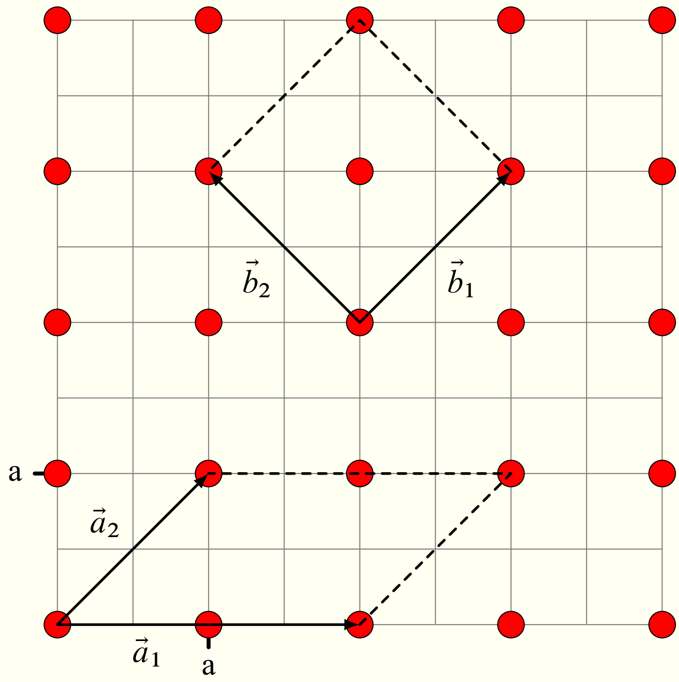
Diamonds form by quite a margin the least dense crystal

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

$$8m_{\text{C}} = \rho V_{\text{dia}}$$
$$r_{\text{dia}}^3 = \frac{3m_{\text{C}}}{\rho\pi 4}$$
$$r_{\text{dia}} = \underline{\underline{1.11 \times 10^{-10} \text{ m}}}$$

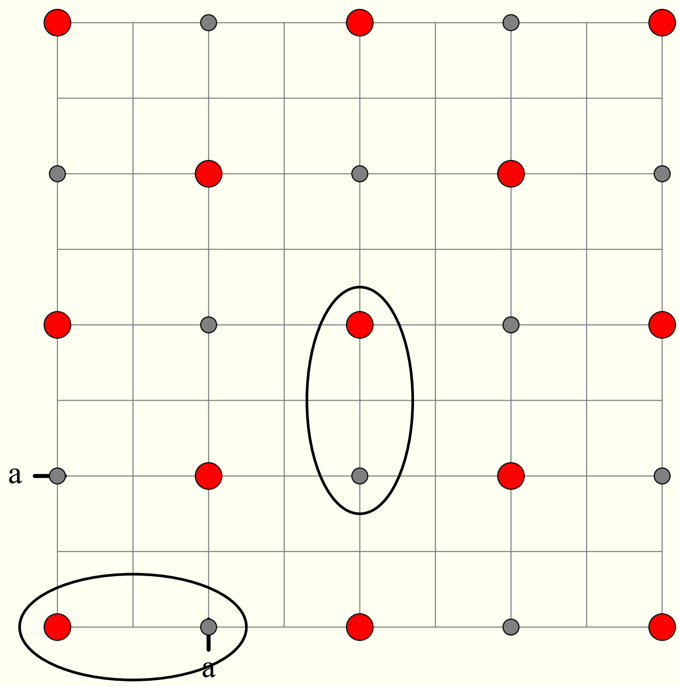
Gitter, Kristallstruktur und Röntgenbeugung

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

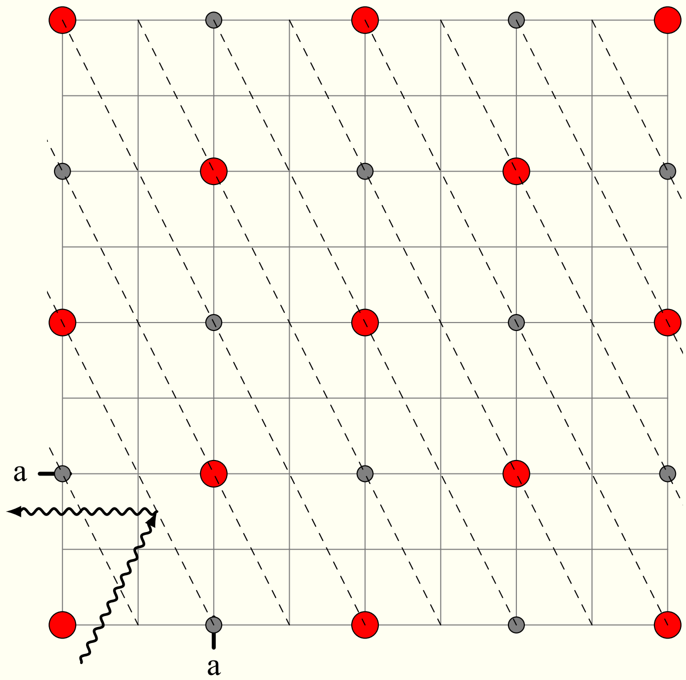


a)

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



b)



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

d) $\lambda = 1.46$ Å; $\quad \theta = 15°$

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

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

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

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

Kristallstruktur von $BaTiO_3$

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

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

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

$$\begin{aligned} d &= \frac{a_0}{\sqrt{1^2+1^2+1^2}} = \frac{a_0}{\sqrt{3}} \\ \lambda_R &= 2d\,\sin(\theta) \\ \theta &= \arcsin\left(\frac{\lambda_R\sqrt{3}}{2a_0}\right) = \underline{\underline{32.77°}} \end{aligned}$$