Diamantstruktur

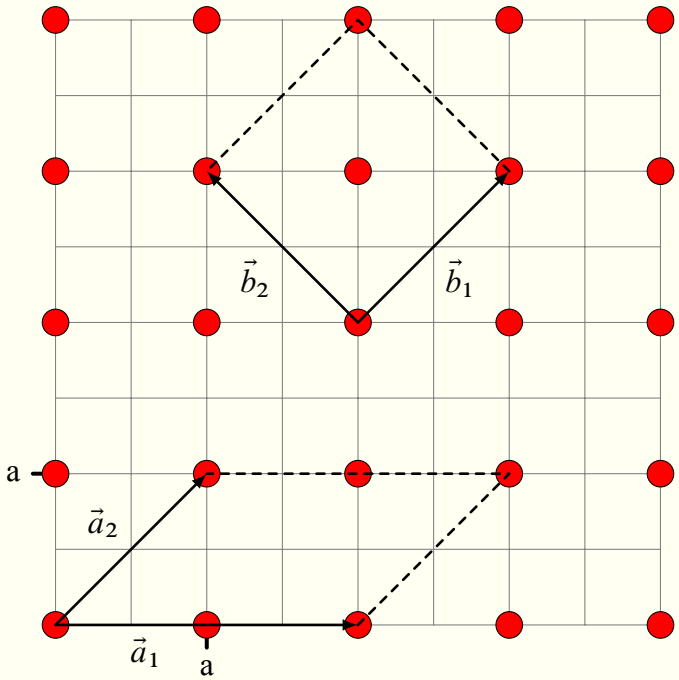
a)

b)

c)

Gitter, Kristallstruktur und Röntgenbeugung

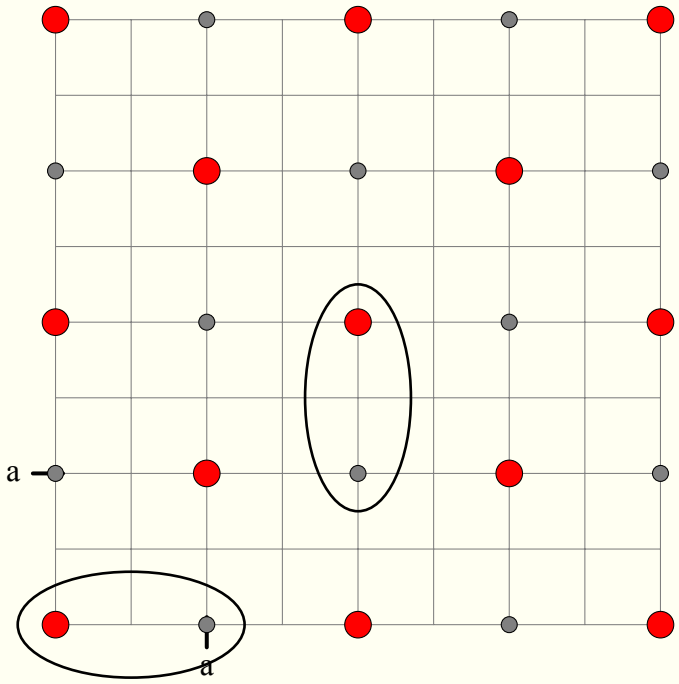
$\vec{a}_1 = 2a\vec{e}_x; \quad \vec{a}_2 = a(\vec{e}_x + \vec{e}_y); \quad \vec{a}_3 = a\vec{e}_z; \quad \vec{r}_A = 0; \quad \vec{r}_B = \vec{a}_1/2$



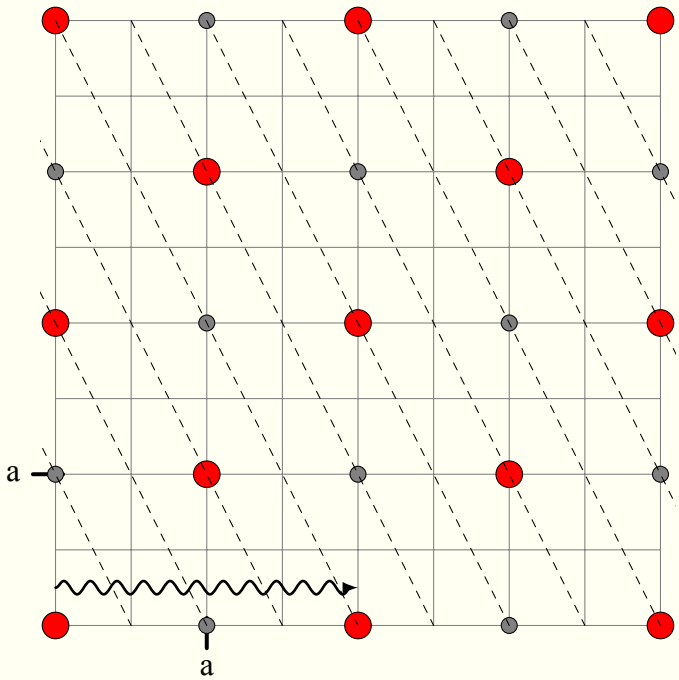
a)

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; $\theta = 15°$

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

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

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 $BaTiO_3$

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

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

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

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

c) $a_0 = 0.4$ nm; $\lambda_R = 0.25$ nm

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