Answer on Question #51235, Physics, Solid State Physics

Task: The direct lattice vectors for a lattice are given by:

$$\vec{a}_1 = a\hat{i};\vec{a}_2 = \frac{a}{2}[\hat{i} + \sqrt{3}\hat{j}];\vec{a}_3 = c\vec{k}$$

Obtain the volume of the primitive cell and the reciprocal lattice vectors.

Answer:

For a given direct lattice we can define a reciprocal lattice in terms of three primitive reciprocal vectors: b_1,b_2 and b_3 which are related to the direct lattice vectors a_1,a_2 and a_3 by $\vec{b}_i = 2\pi\frac{(a_j \times a_k)}{(a_1 \times a_2)\cdot a_3}$, where i,j and k represent a cyclic permutation of the three indices 1,2 and 3 and $(a_1 \times a_2)\cdot a_3$ is the volume of the primitive cell.

So $\vec{a}_1 = (a;0;0);\vec{a}_2 = (\frac{a}{2};\frac{a\sqrt{3}}{2};0);\vec{a}_3 = (0;0;c)$

The volume of the primitive cell $V_{cell} = (a_1 \times a_2)\cdot a_3 = \begin{vmatrix} a & 0 & 0 \\ \frac{a}{2} & \frac{a\sqrt{3}}{2} & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{a^2}{c}\frac{\sqrt{3}}{2}$

$$\vec{b}_1 = 2\pi\frac{(\vec{a}_2 \times \vec{a}_3)}{V_{cell}} = \frac{2\pi}{\frac{a^2\sqrt{3}}{2c}}\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{a}{2} & \frac{a\sqrt{3}}{2} & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{4\pi c}{a^2\sqrt{3}}[\frac{ac\sqrt{3}}{2}\hat{i} - \frac{ac}{2}\hat{j}] = \frac{4\pi c^2}{2a\sqrt{3}}[\sqrt{3}\hat{i} - \hat{j}]$$

$$\vec{b}_2 = 2\pi\frac{(\vec{a}_1 \times \vec{a}_3)}{V_{cell}} = \frac{2\pi}{\frac{a^2\sqrt{3}}{2c}}\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ a & 0 & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{4\pi c}{a^2\sqrt{3}}[-ac\hat{j}] = -\frac{4\pi c^2}{a\sqrt{3}}\hat{j}$$

$$\vec{b}_3 = 2\pi\frac{(\vec{a}_2 \times \vec{a}_1)}{V_{cell}} = \frac{2\pi}{\frac{a^2\sqrt{3}}{2c}}\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{a}{2} & \frac{a\sqrt{3}}{2} & 0 \\ a & 0 & 0 \end{vmatrix} = \frac{4\pi c}{a^2\sqrt{3}}[\frac{a^2\sqrt{3}}{2}\hat{k}] = 2\pi c\hat{k}$$