



Direct lattice vectors of a simple hexagonal

Bravais lattice :

$$\begin{cases} \vec{R}_1 = \frac{\sqrt{3}}{2} a \hat{x} + \frac{1}{2} a \hat{y} \\ \vec{R}_2 = -\frac{\sqrt{3}}{2} a \hat{x} + \frac{1}{2} a \hat{y} \\ \vec{R}_3 = c \hat{z} \end{cases}$$

$$\vec{R}_1 \cdot \vec{R}_2 \times \vec{R}_3 = \begin{vmatrix} \frac{\sqrt{3}}{2} a & \frac{1}{2} a & 0 \\ -\frac{\sqrt{3}}{2} a & \frac{1}{2} a & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{\sqrt{3}}{2} a^2 c$$

$$\vec{R}_2 \times \vec{R}_3 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -\frac{\sqrt{3}}{2} a & \frac{1}{2} a & 0 \\ 0 & 0 & c \end{vmatrix} = \left(\frac{1}{2} ac\right) \hat{x} + \left(\frac{\sqrt{3}}{2} ac\right) \hat{y}$$

$$\vec{R}_3 \times \vec{R}_1 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ \frac{\sqrt{3}}{2} a & \frac{1}{2} a & 0 \end{vmatrix} = \left(-\frac{1}{2} ac\right) \hat{x} + \left(\frac{\sqrt{3}}{2} ac\right) \hat{y}$$

$$\vec{R}_1 \times \vec{R}_2 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\sqrt{3}}{2} a & \frac{1}{2} a & 0 \\ -\frac{\sqrt{3}}{2} a & \frac{1}{2} a & 0 \end{vmatrix} = \frac{\sqrt{3}}{2} a^2 \hat{z}$$

⇒ Reciprocal lattice vectors :

$$\vec{G}_1 = 2\pi \frac{\vec{R}_2 \times \vec{R}_3}{\vec{R}_1 \cdot (\vec{R}_2 \times \vec{R}_3)} = 2\pi \frac{\left(\frac{1}{2} ac\right) \hat{x} + \left(\frac{\sqrt{3}}{2} ac\right) \hat{y}}{\frac{\sqrt{3}}{2} a^2 c} = \frac{2\pi}{\sqrt{3} a} \hat{x} + \frac{2\pi}{a} \hat{y}$$