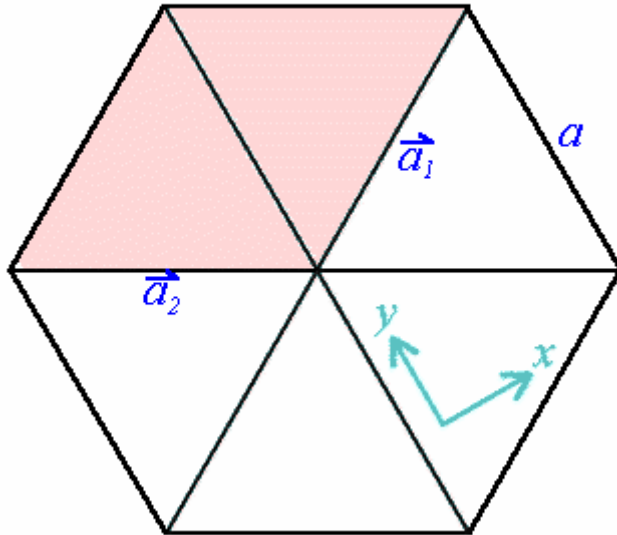


Kittel (7<sup>th</sup> Edition). Chapter 2. Problem 2.  
© Kwok-Wai Ng, 2005.

■ Unit cell



$$(a) \text{ Area of the hexagonal base} = 2 \times \left( \frac{a \times \frac{\sqrt{3}}{2} a}{2} \right) = \frac{\sqrt{3} a^2}{2}$$

$$\therefore \text{ Volume of cell} = \text{Area of base} \times \text{height} = \underline{\underline{\frac{\sqrt{3} a^2 c}{2}}}$$

$$\begin{aligned}
 \text{(b) } \bar{\mathbf{b}}_1 &= \frac{2\pi}{V} \bar{\mathbf{a}}_2 \times \bar{\mathbf{a}}_3 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -\frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{2\pi \times 2}{\sqrt{3}a^2c} \left( \frac{ac}{2} \hat{x} + \frac{ac\sqrt{3}}{2} \hat{y} \right) \\
 &= \frac{2\pi}{\sqrt{3}a} \hat{x} + \frac{2\pi}{a} \hat{y}
 \end{aligned}$$

$$\begin{aligned}
 \bar{\mathbf{b}}_2 &= \frac{2\pi}{V} \bar{\mathbf{a}}_3 \times \bar{\mathbf{a}}_1 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ \frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \end{vmatrix} = \frac{2\pi \times 2}{\sqrt{3}a^2c} \left( -\frac{ac}{2} \hat{x} + \frac{ac\sqrt{3}}{2} \hat{y} \right) \\
 &= -\frac{2\pi}{\sqrt{3}a} \hat{x} + \frac{2\pi}{a} \hat{y}
 \end{aligned}$$

$$\begin{aligned}
 \bar{\mathbf{b}}_3 &= \frac{2\pi}{V} \bar{\mathbf{a}}_1 \times \bar{\mathbf{a}}_2 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ -\frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \end{vmatrix} = \frac{2\pi \times 2}{\sqrt{3}a^2c} \left( \frac{\sqrt{3}a^2}{4} + \frac{\sqrt{3}a^2}{4} \right) \hat{z} \\
 &= \frac{2\pi}{c} \hat{z}
 \end{aligned}$$

The reciprocal lattice is the same as the original lattice, with lattice parameter  $\frac{4\pi}{a}, \frac{4\pi}{a}, \frac{2\pi}{c}$ .

(c)

