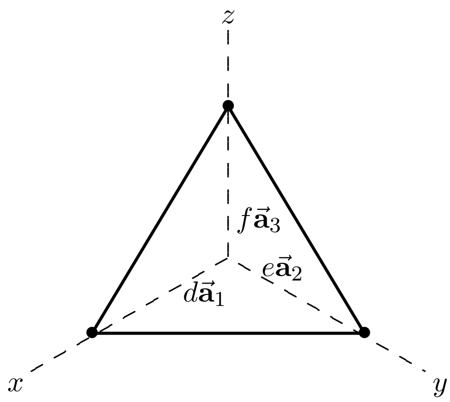
Solutions
Chapter 2

Problem 1

Part a



Let $\{def\}$ be the smallest intercepts as multiples of the three lattice parameters representing a given set of planes. The inverses of these are $\{1/d, 1/e, 1/f\}$. Multiplying this by m, the LCM of $\{def\}$, gives the Miller indices:

$$(hkl) = \left(\frac{m}{d} \frac{m}{e} \frac{m}{f} \right). \tag{1}$$

Note that m is also the LCM of (hkl).

Consider the two following vectors given by two sides of the triangle in the plane (see figure above).

$$\vec{\mathbf{R}}_1 = e\vec{\mathbf{a}}_2 - f\vec{\mathbf{a}}_3, \quad \vec{\mathbf{R}}_2 = f\vec{\mathbf{a}}_3 - d\vec{\mathbf{a}}_1. \tag{2}$$

For the given vector

$$\vec{\mathbf{G}} = h\vec{\mathbf{b}}_1 + k\vec{\mathbf{b}}_2 + l\vec{\mathbf{b}}_3, \tag{3}$$

it is seen that

$$\vec{\mathbf{G}} \cdot \vec{\mathbf{R}}_1 = 2\pi ek - 2\pi fl = 0, \tag{4}$$

as equation 1 gives $ek = fl = m$. Similarly,

$$\vec{\mathbf{G}} \cdot \vec{\mathbf{R}}_2 = 2\pi fl - 2\pi dh = 0, \tag{5}$$

This shows that $\vec{\mathbf{G}}$ is perpendicular to both $\vec{\mathbf{R}}_1$ and $\vec{\mathbf{R}}_2$. Hence, $\vec{\mathbf{G}}$ is perpendicular to the plane. A unit vector along this perpendicular is given by

$$\hat{\mathbf{n}} = \frac{\vec{\mathbf{G}}}{|\vec{\mathbf{G}}|}. \tag{6}$$

Part b

The triangular piece drawn in the figure can be seen to be the mth plane of the given set of planes starting from the origin. This can be visualized by noticing that a crystal plane parallel to the triangle must pass through every lattice point on the three axis between the triangle and the origin. So, a plane must pass through the origin. The next closest plane will intersect the x axis at the point given by $d\vec{\mathbf{a}}_1/m = \vec{\mathbf{a}}_1/h$. The projection of this vector along the perpendicular to the plane gives the distance between the planes. Using the unit vector defined in equation 6, this projection is computed to be

$$d(hkl) = \frac{\vec{\mathbf{a}}_1}{h} \cdot \hat{\mathbf{n}} = \frac{\vec{\mathbf{a}}_1}{h} \cdot \frac{\vec{\mathbf{G}}}{|\vec{\mathbf{G}}|} = \frac{2\pi}{|\vec{\mathbf{G}}|}. \tag{7}$$

Problem 2

Part a

The volume is the triple product of the three primitive translation vectors.

$$V_c = \vec{\mathbf{a}}_1 \cdot (\vec{\mathbf{a}}_2 \times \vec{\mathbf{a}}_3) = \left(\frac{\sqrt{3}a\hat{\mathbf{x}}}{2} + \frac{a\hat{\mathbf{y}}}{2}\right) \cdot \left(\left(-\frac{\sqrt{3}a\hat{\mathbf{x}}}{2} + \frac{a\hat{\mathbf{y}}}{2}\right) \times (c\hat{\mathbf{z}})\right)$$

$$= \left(\frac{\sqrt{3}a\hat{\mathbf{x}}}{2} + \frac{a\hat{\mathbf{y}}}{2}\right) \cdot \left(\frac{ac\hat{\mathbf{x}}}{2} + \frac{\sqrt{3}ac\hat{\mathbf{y}}}{2}\right) = \frac{\sqrt{3}a^2c}{2}.$$

Part b

$$\vec{\mathbf{a}}_2 \times \vec{\mathbf{a}}_3 = \left(-\frac{\sqrt{3}a\hat{\mathbf{x}}}{2} + \frac{a\hat{\mathbf{y}}}{2}\right) \times (c\hat{\mathbf{z}}) = \frac{ac\hat{\mathbf{x}}}{2} + \frac{\sqrt{3}ac\hat{\mathbf{y}}}{2}.$$

$$\vec{\mathbf{b}}_1 = \frac{2\pi\vec{\mathbf{a}}_2 \times \vec{\mathbf{a}}_3}{V_c} = \frac{2\pi\hat{\mathbf{x}}}{\sqrt{3}a} + \frac{2\pi\hat{\mathbf{y}}}{a}.$$

$$\vec{\mathbf{a}}_3 \times \vec{\mathbf{a}}_1 = (c\hat{\mathbf{z}}) \times \left(\frac{\sqrt{3}a\hat{\mathbf{x}}}{2} + \frac{a\hat{\mathbf{y}}}{2}\right) = -\frac{ac\hat{\mathbf{x}}}{2} + \frac{\sqrt{3}ac\hat{\mathbf{y}}}{2}.$$

$$\vec{\mathbf{b}}_2 = \frac{2\pi\vec{\mathbf{a}}_3 \times \vec{\mathbf{a}}_1}{V_c} = -\frac{2\pi\hat{\mathbf{x}}}{\sqrt{3}a} + \frac{2\pi\hat{\mathbf{y}}}{a}.$$

$$\vec{\mathbf{a}}_1 \times \vec{\mathbf{a}}_2 = \left(\frac{\sqrt{3}a\hat{\mathbf{x}}}{2} + \frac{a\hat{\mathbf{y}}}{2}\right) \times \left(-\frac{\sqrt{3}a\hat{\mathbf{x}}}{2} + \frac{a\hat{\mathbf{y}}}{2}\right) = \frac{\sqrt{3}a^2\hat{\mathbf{z}}}{2}.$$

$$\vec{\mathbf{b}}_3 = \frac{2\pi\vec{\mathbf{a}}_1 \times \vec{\mathbf{a}}_2}{V_c} = \frac{2\pi\hat{\mathbf{z}}}{c}.$$

Problem 3

Volume of Brillouin zone is

$$V_b = \vec{\mathbf{b}}_1 \cdot (\vec{\mathbf{b}}_2 \times \vec{\mathbf{b}}_3) = (2\pi/V_c)^3(\vec{\mathbf{a}}_2 \times \vec{\mathbf{a}}_3) \cdot ((\vec{\mathbf{a}}_3 \times \vec{\mathbf{a}}_1) \times (\vec{\mathbf{a}}_1 \times \vec{\mathbf{a}}_2))$$

$$= (2\pi/V_c)^3(\vec{\mathbf{a}}_2 \times \vec{\mathbf{a}}_3) \cdot (\vec{\mathbf{a}}_3 \cdot (\vec{\mathbf{a}}_1 \times \vec{\mathbf{a}}_2)\vec{\mathbf{a}}_1) = (2\pi/V_c)^3(\vec{\mathbf{a}}_2 \times \vec{\mathbf{a}}_3) \cdot (V_c\vec{\mathbf{a}}_1) = (2\pi/V_c)^3 V_c(\vec{\mathbf{a}}_2 \times \vec{\mathbf{a}}_3) \cdot \vec{\mathbf{a}}_1$$

$$= (2\pi/V_c)^3 V_c^2 = (2\pi)^3/V_c.$$