CHAPTER 2

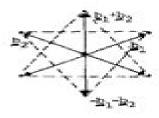
1. The crystal plane with Miller indices $hk\ell$ is a plane defined by the points a_0h , a_0k , and $a_1 \neq \ell$. (a) Two vectors that lie in the plane may be taken as $a_0h - a_0k$ and $a_1 \neq h - a_3 \neq \ell$. But each of these vectors gives zero as its scalar product with $G = ha_1 + ka_2 + \ell a_3$, so that G must be perpendicular to the plane $hk\ell$. (b) If $\hat{\mathbf{n}}$ is the unit normal to the plane, the interplanar spacing is $\hat{\mathbf{n}} \cdot \mathbf{a}_1/h$. But $\hat{\mathbf{n}} = G/1G I$, whence $d(hk\ell) = G \cdot a_1/h(G) = 2\pi/1G I$. (c) For a simple cubic lattice $G = (2\pi/a)(h\hat{\mathbf{x}} + k\hat{\mathbf{y}} + \ell\hat{\mathbf{z}})$, whence

$$\frac{1}{\mathbf{d}^2} = \frac{G^2}{4\pi^2} = \frac{h^2 + k^2 + \ell^2}{a^2} \ .$$

2. (a) Cell volume
$$\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_5 = \begin{vmatrix} \frac{1}{2}\sqrt{3}a & \frac{1}{2}a & 0 \\ -\frac{1}{2}\sqrt{3}a & \frac{1}{2}a & 0 \\ 0 & 0 & c \end{vmatrix}$$

$$=\frac{1}{2}\sqrt{3}a^{2}c$$
.

(b)
$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{|\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3|} = \frac{4\pi}{\sqrt{3}a^2c} \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ -\frac{1}{2}\sqrt{3}a & \frac{1}{2}a & 0 \\ 0 & 0 & c \end{vmatrix}$$
$$= \frac{2\pi}{a} (\frac{1}{\sqrt{3}}\hat{\mathbf{x}} + \hat{\mathbf{y}}), \text{ and similarly for } \mathbf{b}_2, \mathbf{b}_3.$$



- (c) Six vectors in the reciprocal lattice are shown as solid lines. The broken lines are the perpendicular bisectors at the midpoints. The inscribed hexagon forms the first Brillouin Zone.
- 3. By definition of the primitive reciprocal lattice vectors

$$\begin{split} V_{\text{BZ}} &= (2\pi)^3 \frac{(a_2 \times a_3) \cdot (a_3 \times a_1) \times (a_1 \times a_2)}{\|(a_1 \cdot a_2 \times a_3)^3\|} = (2\pi)^3 / \|(a_1 \cdot a_2 \times a_3)\| \\ &= (2\pi)^3 / V_{\text{C}}. \end{split}$$

For the vector identity, see G. A. Korn and T. M. Korn, Mathematical handbook for scientists and engineers, McGraw-Hill, 1961, p. 147.

4. (a) This follows by forming

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