CHAPTER 2

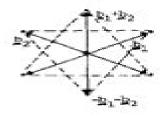
1. The crystal plane with Miller indices $hk\ell$ is a plane defined by the points a_0h , a_0k , and $a_1 \neq \ell$. (a) Two vectors that lie in the plane may be taken as $a_0h - a_0k$ and $a_1 \neq h - a_3 \neq \ell$. But each of these vectors gives zero as its scalar product with $G = ha_1 + ka_2 + \ell a_3$, 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
$$\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_5 = \begin{vmatrix} \frac{1}{2}\sqrt{3}a & \frac{1}{2}a & 0 \\ -\frac{1}{2}\sqrt{3}a & \frac{1}{2}a & 0 \\ 0 & 0 & c \end{vmatrix}$$

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

(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

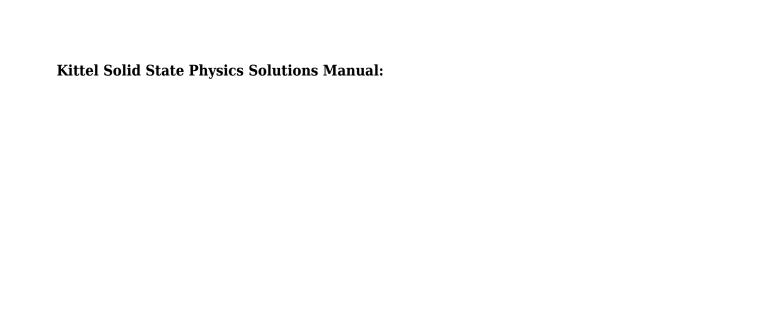
$$\begin{split} V_{\text{BZ}} &= (2\pi)^3 \frac{(a_2 \times a_3) \cdot (a_3 \times a_1) \times (a_1 \times a_2)}{\|(a_1 \cdot a_2 \times a_3)^3\|} = (2\pi)^3 / \|(a_1 \cdot a_2 \times a_3)\| \\ &= (2\pi)^3 / V_{\text{C}}. \end{split}$$

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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