

CHAPTER 2

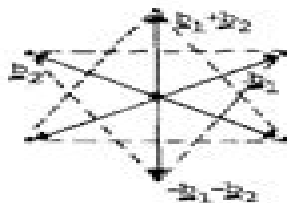
1. The crystal plane with Miller indices hkl is a plane defined by the points \mathbf{a}_1/h , \mathbf{a}_2/k , and \mathbf{a}_3/ℓ . (a) Two vectors that lie in the plane may be taken as $\mathbf{a}_1/h - \mathbf{a}_2/k$ and $\mathbf{a}_1/h - \mathbf{a}_3/\ell$. But each of these vectors gives zero as its scalar product with $\mathbf{G} = h\mathbf{a}_1 + k\mathbf{a}_2 + \ell\mathbf{a}_3$, so that \mathbf{G} must be perpendicular to the plane hkl . (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 $\hat{\mathbf{n}} = \mathbf{G}/|\mathbf{G}|$, whence $d(hkl) = \mathbf{G} \cdot \mathbf{a}_1/h/|\mathbf{G}| = 2\pi/|\mathbf{G}|$. (c) For a simple cubic lattice $\mathbf{G} = (2\pi/a)(h\hat{\mathbf{x}} + k\hat{\mathbf{y}} + \ell\hat{\mathbf{z}})$, whence

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

$$2. (a) \text{ Cell volume } \mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3 = \begin{vmatrix} \frac{1}{2}\sqrt{3}a & \frac{1}{2}a & 0 \\ -\frac{1}{2}\sqrt{3}a & \frac{1}{2}a & 0 \\ 0 & 0 & c \end{vmatrix}$$

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

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



(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

$$\mathbf{V}_{\text{rec}} = (2\pi)^3 \frac{(\mathbf{a}_2 \times \mathbf{a}_3) \cdot (\mathbf{a}_3 \times \mathbf{a}_1) \times (\mathbf{a}_1 \times \mathbf{a}_2)}{|\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3|^3} = (2\pi)^3 / |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| \\ = (2\pi)^3 / V_C.$$

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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Chih-Tang Sah



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