**CHAPTER 2**

1. The crystal plane with Miller indices $hk\ell$ is a plane defined by the points $\mathbf{a}_1/h$, $\mathbf{a}_2/k$, and $\mathbf{a}_3/\ell$. (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 $hk\ell$. (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 $\hat{\mathbf{n}} = \mathbf{G}/|\mathbf{G}|$, whence $d(hk\ell) = G \cdot \mathbf{a}_1/h|\mathbf{G}| = 2\pi/|G|$. (c) For a simple cubic lattice $\mathbf{G} = (2\pi/a)(h\hat{\mathbf{x}} + k\hat{\mathbf{y}} + \ell\hat{\mathbf{z}})$, whence

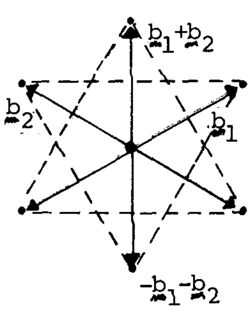
$$\frac{1}{d^2} = \frac{G^2}{4\pi^2} = \frac{h^2 + k^2 + \ell^2}{a^2} .$$

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

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

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

$$= \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{\mathbf{x}} + \hat{\mathbf{y}}\right), \text{ and similarly for } \mathbf{b}_2,\ \mathbf{b}_3.$$




(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

$$V_{BZ} = (2\pi)^3 \frac{(a_2 \times a_3) \cdot (a_3 \times a_1) \times (a_1 \times a_2)}{|(a_1 \cdot a_2 \times a_3)^3|} = (2\pi)^3 / |(a_1 \cdot a_2 \times a_3)|$$

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

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

$$|F|^2 = \frac{1-\exp[-iM(a\cdot\Delta k)]}{1-\exp[-i(a\cdot\Delta k)]}\cdot\frac{1-\exp[iM(a\cdot\Delta k)]}{1-\exp[i(a\cdot\Delta k)]}$$
$$= \frac{1-\cos M(a\cdot\Delta k)}{1-\cos(a\cdot\Delta k)} = \frac{\sin^2 \frac{1}{2}M(a\cdot\Delta k)}{\sin^2\frac{1}{2}(a\cdot\Delta k)}.$$

(b) The first zero in $\sin\frac{1}{2}M\varepsilon$ occurs for ε = 2π/M. That this is the correct consideration follows from

$$\sin M(\pi h + \frac{1}{2}\varepsilon) = \underbrace{\sin \pi Mh}_{\substack{\text{zero,}\\ \text{as Mh is}\\ \text{an integer}}} \cos \frac{1}{2}M\varepsilon + \underbrace{\cos \pi Mh}_{\pm 1} \sin\frac{1}{2}M\varepsilon.$$

5. $S\,(v_1v_2v_3) = f\sum_j e^{-2\pi i(x_jv_1+y_jv_2+z_jv_3)}$

Referred to an fcc lattice, the basis of diamond is $000;\ \frac{1}{4}\frac{1}{4}\frac{1}{4}.$ Thus in the product

$$S(v_1v_2v_3) = S(\text{fcc lattice}) \times S\,(\text{basis}),$$

we take the lattice structure factor from (48), and for the basis

$$S\,(\text{basis}) = 1 + e^{-i\frac{1}{2}\pi(v_1+v_2+v_3).}$$

Now S(fcc) = 0 only if all indices are even or all indices are odd. If all indices are even the structure factor of the basis vanishes unless $v_1 + v_2 + v_3 = 4n$, where n is an integer. For example, for the reflection (222) we have S(basis) = 1 + $e^{-i3\pi}$ = 0, and this reflection is forbidden.

6.
$$f_G = \int_0^\infty 4\pi r^2\,(\pi a_0{}^3\ Gr)^{-1}\ \sin Gr\ \exp\,(-2r/a_0)\ dr$$
$$= (4/G^3a_0{}^3)\int dx\ x\ \sin x\ \exp\,(-2x/Ga_0)$$
$$= (4/G^3a_0{}^3)\ (4/Ga_0)/(1+r/G^2a_0{}^2)^2$$
$$16/(4+G^2a_0{}^2)^2.$$

The integral is not difficult; it is given as Dwight 860.81. Observe that f = 1 for G = 0 and $f \propto 1/G^4$ for $Ga_0 >> 1$.

7. (a) The basis has one atom A at the origin and one atom B at $\frac{1}{2}$a. The single Laue equation $\mathbf{a}\cdot\Delta\mathbf{k} = 2\pi\times$ (integer) defines a set of parallel planes in Fourier space. Intersections with a sphere are a set of circles, so that the diffracted beams lie on a set of cones. (b) S(n) = $f_A + f_B\, e^{-i\pi n}$. For n odd, S = $f_A$ –

$f_B$; for n even, $S = f_A + f_B$. (c) If $f_A = f_B$ the atoms diffract identically, as if the primitive translation vector were $\frac{1}{2}$ a and the diffraction condition $(\frac{1}{2}\mathbf{a} \cdot \Delta\mathbf{k}) = 2\pi \times (\text{integer})$.