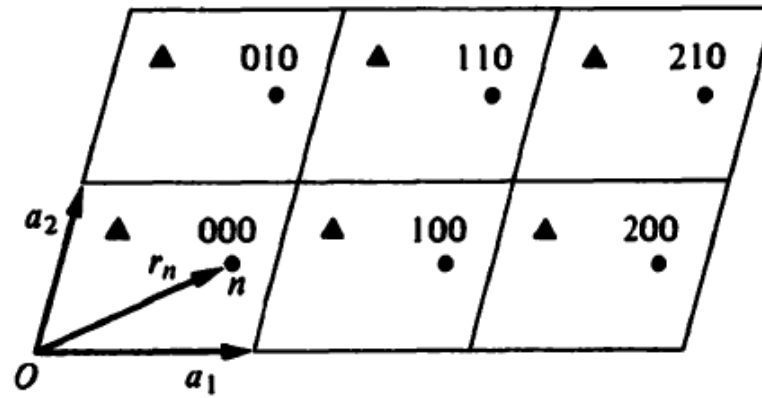


Fig. 5. Atomic scattering factors  $f$  for hydrogen, carbon and fluorine, plotted against  $\sin \theta/\lambda$ .

# Crystal Axes and Reciprocal Lattice

Text from B. E Warren, Chapter 2



We suppose that the different atoms in the unit cell are numbered  $1, 2, 3, \dots, n$ , and that the positions of the atoms relative to the cell origin are given by cell vectors  $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_n$ . We shall designate the different unit cells by three integers  $m_1, m_2, m_3$ , such that cell  $m_1 m_2 m_3$  is the one whose origin is displaced from the crystal origin by  $m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3$ . Finally the position of the atom of type  $n$  in the unit cell  $m_1 m_2 m_3$  is given by the vector

$$\mathbf{R}_m^n = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3 + \mathbf{r}_n. \quad (2.1)$$

## 2.2 THE CRYSTALLOGRAPHIC PLANES $hkl$

In using the Bragg law, we consider diffraction in terms of a set of crystallographic planes  $hkl$ . A precise definition of this concept is indicated by Fig. 2.2. By the set of crystallographic planes  $hkl$ , we mean a set of parallel equidistant planes, one of which passes through the origin, and the next nearest makes intercepts  $a_1/h$ ,  $a_2/k$ , and  $a_3/l$  on the three crystallographic axes. The integers  $hkl$  are usually called the Miller indices.

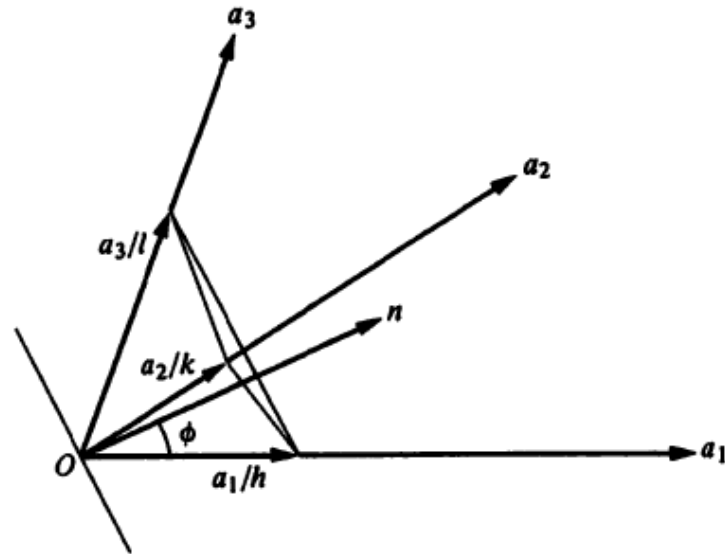


Fig. 2.2 Representation of the crystallographic planes  $hkl$ .

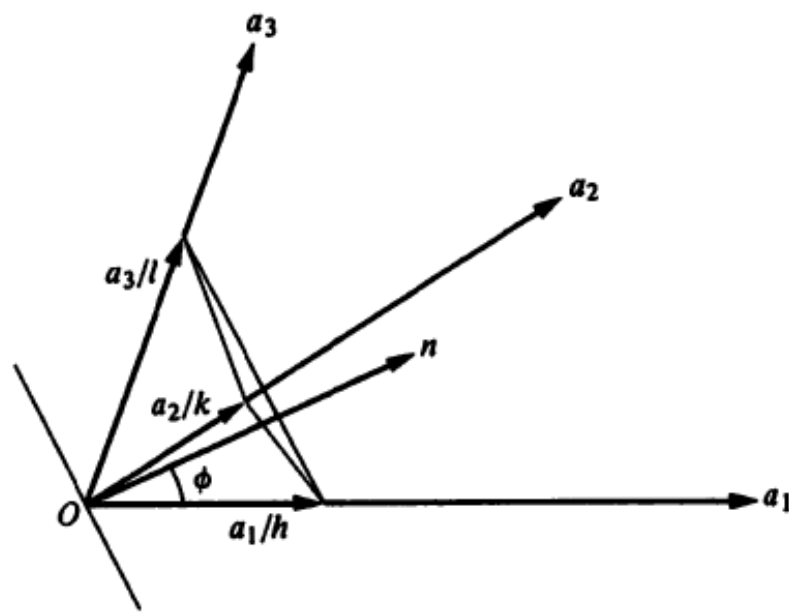
### 2.3 RECIPROCAL VECTORS AND THE RECIPROCAL LATTICE

In terms of the crystal axes  $\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3$ , we define a set of reciprocal vectors  $\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3$ :

$$\mathbf{b}_1 = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}, \quad \mathbf{b}_2 = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}, \quad \mathbf{b}_3 = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}. \quad (2.2)$$

$$\mathbf{a}_i \cdot \mathbf{b}_j = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

$$\mathbf{H}_{hkl} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3.$$



**Fig. 2.2** Representation of the crystallographic planes  $hkl$ .

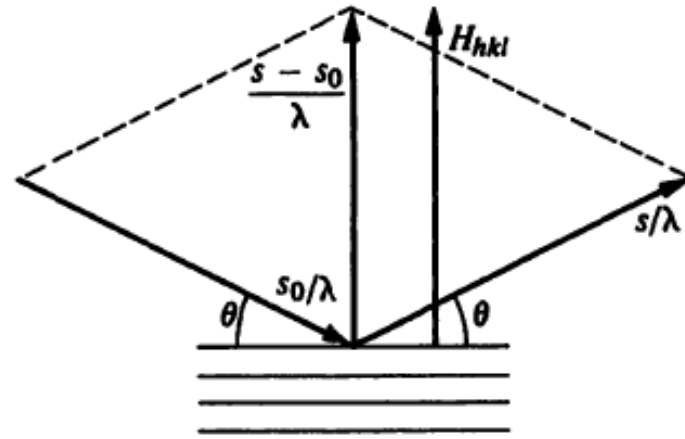
From Fig. 2.2 it is evident that  $(\mathbf{a}_1/h - \mathbf{a}_2/k)$  and  $(\mathbf{a}_2/k - \mathbf{a}_3/l)$  are vectors which are parallel to the  $hkl$ -planes. But from the relations expressed by Eq. (2.3),

$$\left(\frac{\mathbf{a}_1}{h} - \frac{\mathbf{a}_2}{k}\right) \cdot \mathbf{H}_{hkl} = \left(\frac{\mathbf{a}_1}{h} - \frac{\mathbf{a}_2}{k}\right) \cdot (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) = 1 - 1 = 0,$$

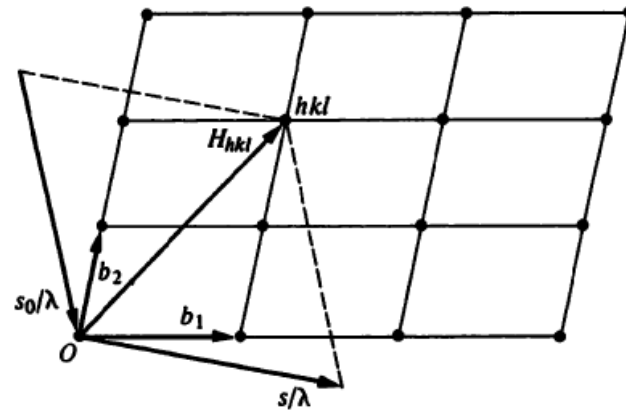
$$\left(\frac{\mathbf{a}_2}{k} - \frac{\mathbf{a}_3}{l}\right) \cdot \mathbf{H}_{hkl} = \left(\frac{\mathbf{a}_2}{k} - \frac{\mathbf{a}_3}{l}\right) \cdot (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) = 1 - 1 = 0.$$

Since  $\mathbf{H}_{hkl}$  is perpendicular to the  $hkl$ -planes, we can make up a unit vector  $\mathbf{n}$  by using  $\mathbf{H}_{hkl}/|\mathbf{H}_{hkl}|$ . Hence the spacing is given by

$$d_{hkl} = \frac{a_1}{h} \cdot \frac{(hb_1 + kb_2 + lb_3)}{|\mathbf{H}_{hkl}|} = \frac{1}{|\mathbf{H}_{hkl}|}.$$



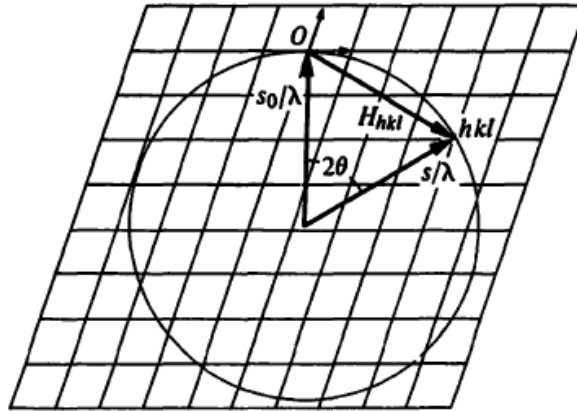
**Fig. 2.3** Relations involved in the vector representation of the Bragg law.



**Fig. 2.4** Reciprocal lattice representation of the satisfying of the Bragg law for a set of planes  $hkl$ . The diffraction vector  $(s - s_0)/\lambda$  must terminate on the point  $hkl$  of the reciprocal lattice.



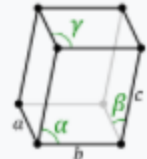
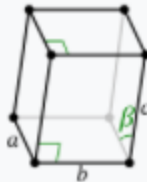
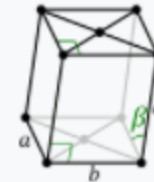
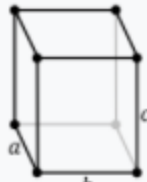



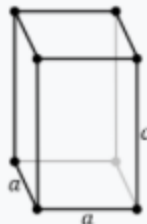
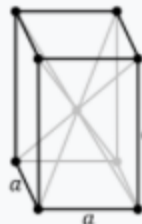
A very powerful and useful way of representing the satisfying of the Bragg law is given by the sphere of reflection (Ewald sphere). The reciprocal lattice is represented schematically in 2 dimensions by Fig. 2.5. The direction of the primary beam is shown by the vector  $s_0/\lambda$ , a vector of length  $1/\lambda$  terminating on the origin of the reciprocal lattice. A sphere of radius  $1/\lambda$  centered on the initial end of  $s_0/\lambda$  passes through the origin. Any reciprocal lattice point  $hkl$  which happens to fall on the surface of the sphere, represents a set of planes  $hkl$  for which the Bragg law is satisfied. The direction of the diffracted beam is given by the vector  $s/\lambda$  from the center of the sphere to the point  $hkl$ . It is evident that the relation of the three vectors  $s_0/\lambda$ ,  $s/\lambda$ , and  $H_{hkl}$  shown by Fig. 2.5 is that of the Bragg law expressed by Eq. (2.5). Although Fig. 2.5 shows the relations schematically in two dimensions, the sphere of reflection construction is valid in three dimensions, and the point  $hkl$  can be anywhere on the surface of the sphere.



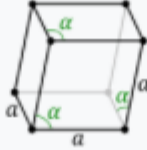
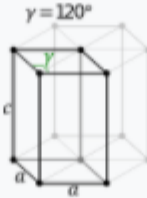
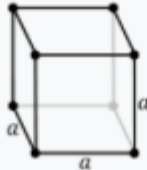
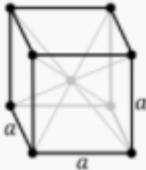

**Fig. 2.5** Two-dimensional representation of the sphere of reflection in the reciprocal lattice. The Bragg law is satisfied for any set of planes whose point  $hkl$  falls on the surface of the sphere.

$$\begin{aligned}
\frac{1}{d_{hkl}^2} &= \frac{a_1^2 a_2^2 a_3^2}{v_a^2} \left\{ \frac{h^2 \sin^2 \alpha_{23}}{a_1^2} + \frac{k^2 \sin^2 \alpha_{31}}{a_2^2} + \frac{l^2 \sin^2 \alpha_{12}}{a_3^2} \right. \\
&\quad + \frac{2hk}{a_1 a_2} (\cos \alpha_{23} \cos \alpha_{31} - \cos \alpha_{12}) + \frac{2kl}{a_2 a_3} (\cos \alpha_{31} \cos \alpha_{12} - \cos \alpha_{23}) \\
&\quad \left. + \frac{2lh}{a_3 a_1} (\cos \alpha_{12} \cos \alpha_{23} - \cos \alpha_{31}) \right\}. \quad (2.6)
\end{aligned}$$

$$\begin{aligned}
\frac{1}{d_{hkl}^2} &= \frac{1}{(1 + 2 \cos \alpha \cos \beta \cos \gamma - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma)} \\
&\quad \times \left\{ \frac{h^2 \sin^2 \alpha}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2 \sin^2 \gamma}{c^2} + \frac{2hk}{ab} (\cos \alpha \cos \beta - \cos \gamma) \right. \\
&\quad \left. + \frac{2kl}{bc} (\cos \beta \cos \gamma - \cos \alpha) + \frac{2lh}{ac} (\cos \gamma \cos \alpha - \cos \beta) \right\}. \quad (2.8)
\end{aligned}$$

Crystal family	Lattice system	Point group (Schönflies notation)	14 Bravais lattices			
			Primitive (P)	Base-centered (S)	Body-centered (I)	Face-centered (F)
Triclinic (a)		$C_i$	 aP			
Monoclinic (m)		$C_{2h}$	 mP	 mS		
Orthorhombic (o)		$D_{2h}$	 oP	 oS	 oI	 oF
Tetragonal (t)		$D_{4h}$	 tP		 tI	

[https://en.wikipedia.org/wiki/Crystal\\_structure](https://en.wikipedia.org/wiki/Crystal_structure)

Hexagonal (h)	Rhombohedral	$D_{3d}$	 hR			
	Hexagonal	$D_{6h}$	$\gamma = 120^\circ$  hP			
Cubic (c)		$O_h$	 cP	 cI	 cF	

Rhombohedral,  $a = b = c$ ,  $\alpha = \beta = \gamma$ :

$$\frac{1}{d_{hkl}^2} = \frac{(h^2 + k^2 + l^2) \sin^2 \alpha + 2(hk + kl + lh)(\cos^2 \alpha - \cos \alpha)}{a^2(1 + 2 \cos^3 \alpha - 3 \cos^2 \alpha)}. \quad (2.9)$$

Hexagonal,  $a = b$ ,  $\alpha = \beta = 90^\circ$ ,  $\gamma = 120^\circ$ :

$$\frac{1}{d_{hkl}^2} = \frac{4}{3} \left( \frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}. \quad (2.10)$$

Monoclinic,  $\alpha = \gamma = 90^\circ$ :

$$\frac{1}{d_{hkl}^2} = \frac{1}{\sin^2 \beta} \left( \frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right). \quad (2.11)$$

Orthorhombic,  $\alpha = \beta = \gamma = 90^\circ$ :

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}. \quad (2.12)$$

Tetragonal,  $a = b$ ,  $\alpha = \beta = \gamma = 90^\circ$ :

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}. \quad (2.13)$$

Cubic,  $a = b = c$ ,  $\alpha = \beta = \gamma = 90^\circ$ :

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2}. \quad (2.14)$$

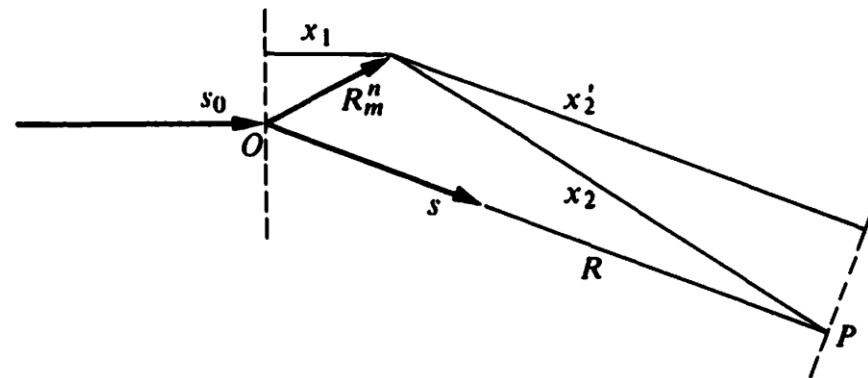
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## Diffraction by a Small Crystal

From B. E Warren, Chapter 3

$$\epsilon_p = \frac{E_0 e^2}{m c^2 R} f_n \cos \left[ 2\pi \nu t - \frac{2\pi}{\lambda} (x_1 + x_2) \right].$$

We assume that the crystal is so small, relative to the distance  $R$  to the point of observation, that the scattered beam can also be treated by the plane-wave



**Fig. 3.1** Diffraction of a parallel primary beam by a small crystal.

$$\epsilon_p = \frac{E_0 e^2}{mc^2 R} f_n e^{i\{2\pi vt - (2\pi/\lambda)[R - (s-s_0) \cdot (m_1 a_1 + m_2 a_2 + m_3 a_3 + r_n)]\}}.$$

$$\begin{aligned} \epsilon_p = \frac{E_0 e^2}{mc^2 R} e^{2\pi i[vt - (R/\lambda)]} \sum_n f_n e^{(2\pi i/\lambda)(s-s_0) \cdot r_n} \sum_{m_1=0}^{N_1-1} e^{(2\pi i/\lambda)(s-s_0) \cdot m_1 a_1} \\ \times \sum_{m_2=0}^{N_2-1} e^{(2\pi i/\lambda)(s-s_0) \cdot m_2 a_2} \sum_{m_3=0}^{N_3-1} e^{(2\pi i/\lambda)(s-s_0) \cdot m_3 a_3}. \end{aligned} \quad (3.1)$$

The summations over  $m_1 m_2 m_3$  have the form of geometric progressions for which the sum is given by

$$S = a + ar + ar^2 + \cdots + l = \frac{rl - a}{r - 1}, \quad (3.3)$$

where  $a$  is the first term,  $l$  is the last term, and  $r$  is the ratio. Using Eq. (3.3), the sum over  $m_1$  becomes

$$\sum_{m_1=0}^{N_1-1} e^{(2\pi i/\lambda)(s-s_0) \cdot m_1 a_1} = \frac{e^{(2\pi i/\lambda)(s-s_0) \cdot N_1 a_1} - 1}{e^{(2\pi i/\lambda)(s-s_0) \cdot a_1} - 1}.$$

With similar expressions for the sums over  $m_2$  and  $m_3$ , the instantaneous field at  $P$  can be written

$$\epsilon_p = \frac{E_0 e^2}{mc^2 R} e^{2\pi i [vt - (R/\lambda)]} F \frac{e^{(2\pi i/\lambda)(s-s_0) \cdot N_1 a_1} - 1}{e^{(2\pi i/\lambda)(s-s_0) \cdot a_1} - 1} \frac{e^{(2\pi i/\lambda)(s-s_0) \cdot N_2 a_2} - 1}{e^{(2\pi i/\lambda)(s-s_0) \cdot a_2} - 1} \times \frac{e^{(2\pi i/\lambda)(s-s_0) \cdot N_3 a_3} - 1}{e^{(2\pi i/\lambda)(s-s_0) \cdot a_3} - 1}.$$



Following the rules set up in Chapter 1, we now write the complex conjugate  $\epsilon_p^*$ :

$$\epsilon_p^* = \frac{E_0 e^2}{m c^2 R} e^{-2\pi i [vt - (R/\lambda)]} F^* \frac{e^{-(2\pi i/\lambda)(s-s_0) \cdot N_1 \mathbf{a}_1} - 1}{e^{-(2\pi i/\lambda)(s-s_0) \cdot \mathbf{a}_1} - 1} \frac{e^{-(2\pi i/\lambda)(s-s_0) \cdot N_2 \mathbf{a}_2} - 1}{e^{-(2\pi i/\lambda)(s-s_0) \cdot \mathbf{a}_2} - 1} \times \frac{e^{-(2\pi i/\lambda)(s-s_0) \cdot N_3 \mathbf{a}_3} - 1}{e^{-(2\pi i/\lambda)(s-s_0) \cdot \mathbf{a}_3} - 1},$$

where by the complex conjugate of the structure factor we mean

$$F^* = \sum_n f_n^* e^{-(2\pi i/\lambda)(s-s_0) \cdot \mathbf{r}_n}. \quad (3.4)$$

In taking the product  $\epsilon_p \epsilon_p^*$ , there will be products of the form

$$\left( \frac{e^{iNx} - 1}{e^{ix} - 1} \right) \left( \frac{e^{-iNx} - 1}{e^{-ix} - 1} \right) = \frac{2 - 2 \cos Nx}{2 - 2 \cos x} = \frac{\sin^2 Nx/2}{\sin^2 x/2}$$

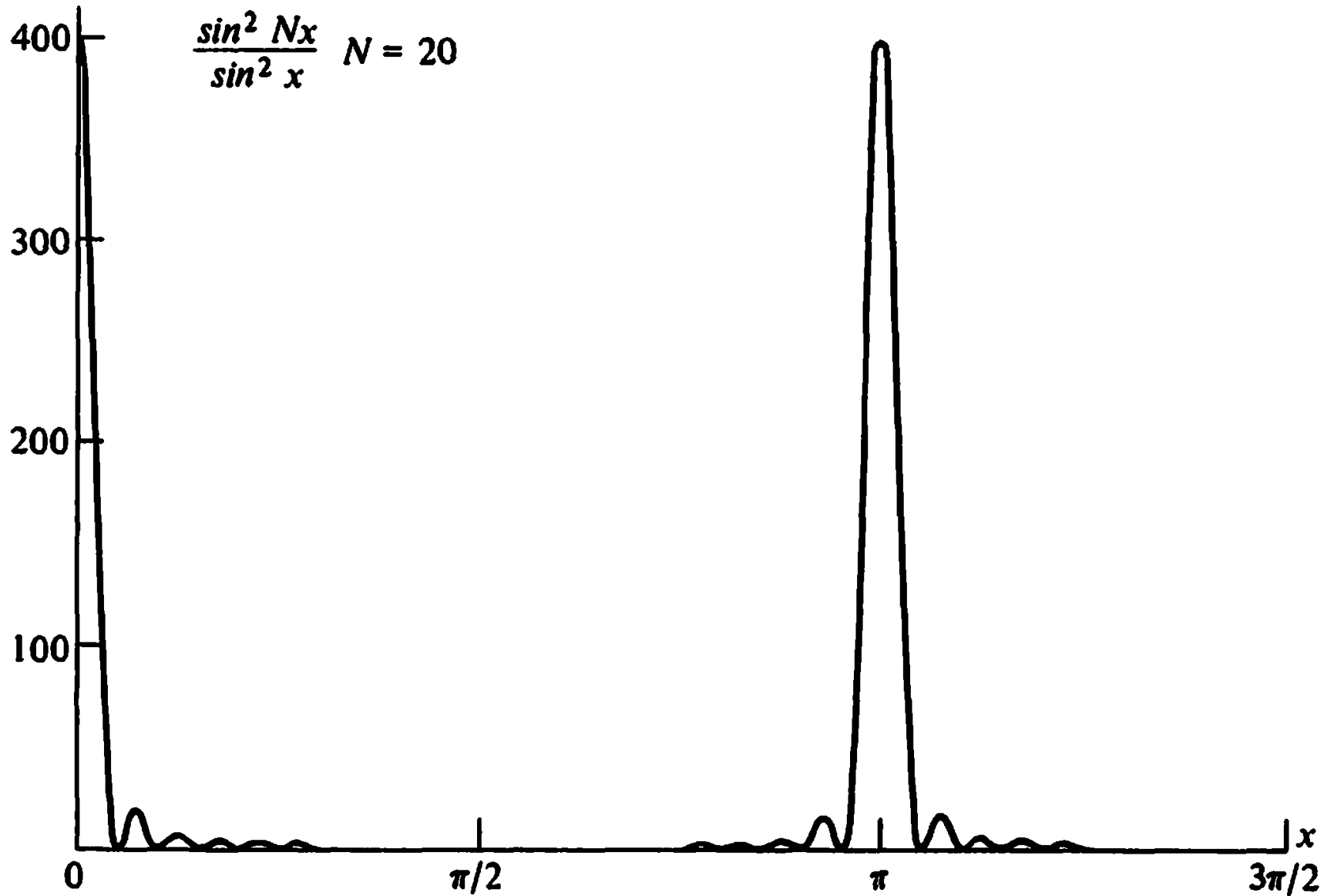
and hence

$$\epsilon_p \epsilon_p^* = \frac{E_0^2 e^4}{m^2 c^4 R^2} F F^* \frac{\sin^2 (\pi/\lambda)(s - s_0) \cdot N_1 \mathbf{a}_1}{\sin^2 (\pi/\lambda)(s - s_0) \cdot \mathbf{a}_1} \frac{\sin^2 (\pi/\lambda)(s - s_0) \cdot N_2 \mathbf{a}_2}{\sin^2 (\pi/\lambda)(s - s_0) \cdot \mathbf{a}_2} \times \frac{\sin^2 (\pi/\lambda)(s - s_0) \cdot N_3 \mathbf{a}_3}{\sin^2 (\pi/\lambda)(s - s_0) \cdot \mathbf{a}_3}. \quad (3.5)$$

$$I_p = I_e F^2 \frac{\sin^2(\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot N_1 \mathbf{a}_1}{\sin^2(\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_1} \frac{\sin^2(\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot N_2 \mathbf{a}_2}{\sin^2(\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_2} \times \frac{\sin^2(\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot N_3 \mathbf{a}_3}{\sin^2(\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_3}, \quad (3.6)$$

where

$$I_e = I_0 \frac{e^4}{m^2 c^4 R^2} \left( \frac{1 + \cos^2 2\theta}{2} \right)$$



**Fig. 3.2** The function  $(\sin^2 Nx)/\sin^2 x$  for  $N = 20$ . The function peaks at values of  $x$  which are integral multiples of  $\pi$ , and it is essentially zero everywhere else.

The value of the intensity at the point of observation depends sharply upon the three quotients of Eq. (3.6). These are of the form

$$y = \frac{\sin^2 Nx}{\sin^2 x},$$

where  $x_i = (\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_i$ . Figure 3.2 shows the function

$$y = \frac{\sin^2 Nx}{\sin^2 x}$$

for  $N = 20$ . The function rises to high maxima  $y = N^2$  at the positions  $x = n\pi$ . For the average crystal which we shall be considering,  $N$  is considerably greater than 20, and the peaks are accordingly much higher and sharper than those of Fig. 3.2. We can say that the function  $y = (\sin^2 Nx)/\sin^2 x$  is essentially zero everywhere except in the immediate vicinity of  $x = n\pi$ , where it rises to high maxima. Hence the intensity  $I_p$  will be essentially zero unless the three quotients are simultaneously close to their maximum values. For  $I_p$  to be a maximum, we must simultaneously satisfy the three conditions

$$(\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_1 = h'\pi,$$

$$(\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_2 = k'\pi,$$

$$(\pi/\lambda)(\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_3 = l'\pi,$$

Since a diffracted beam exists only if the 3 Laue equations are simultaneously satisfied, these three equations together must be equivalent to the Bragg law. To show that this is so, let any arbitrary vector  $\mathbf{r}$  be represented in terms of the three reciprocal vectors:

$$\mathbf{r} = p_1 \mathbf{b}_1 + p_2 \mathbf{b}_2 + p_3 \mathbf{b}_3.$$

To determine the coefficient  $p_1$ , take the scalar product with  $\mathbf{a}_1$ :

$$\mathbf{r} \cdot \mathbf{a}_1 = (p_1 \mathbf{b}_1 + p_2 \mathbf{b}_2 + p_3 \mathbf{b}_3) \cdot \mathbf{a}_1 = p_1.$$

With  $p_2$  and  $p_3$  determined in a similar way, we can write the general relation for expressing a vector  $\mathbf{r}$  in terms of the reciprocal vectors  $\mathbf{b}_1 \mathbf{b}_2 \mathbf{b}_3$ :

$$\mathbf{r} = (\mathbf{r} \cdot \mathbf{a}_1) \mathbf{b}_1 + (\mathbf{r} \cdot \mathbf{a}_2) \mathbf{b}_2 + (\mathbf{r} \cdot \mathbf{a}_3) \mathbf{b}_3. \quad (3.8)$$

We now let  $\mathbf{r}$  be the vector  $(\mathbf{s} - \mathbf{s}_0)$ , and combine Eq. (3.8) with the 3 Laue equations:

$$\begin{aligned} (\mathbf{s} - \mathbf{s}_0) &= (\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_1 \mathbf{b}_1 + (\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_2 \mathbf{b}_2 + (\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{a}_3 \mathbf{b}_3 \\ &= \lambda(h' \mathbf{b}_1 + k' \mathbf{b}_2 + l' \mathbf{b}_3), \quad (3.9) \end{aligned}$$

$$\mathbf{s} - \mathbf{s}_0 = \lambda \mathbf{H}_{h'k'l'}.$$

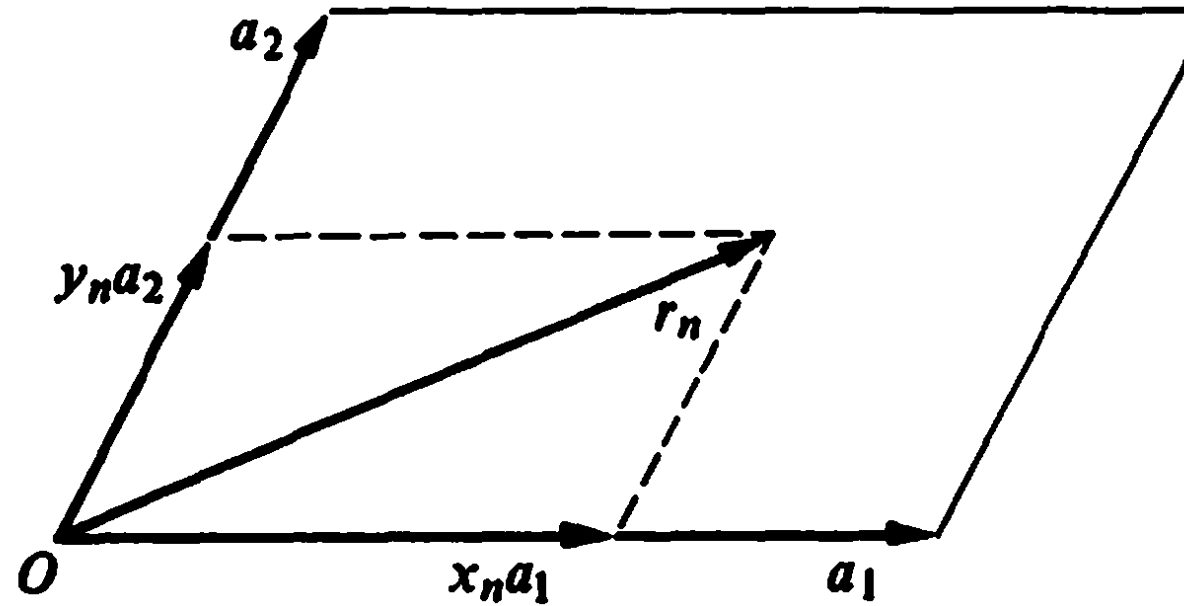
Combining with Eq. (2.5) it is seen that Eq. (3.9) is identical to the Bragg law of

### 3.3 STRUCTURE FACTOR FOR A BRAGG REFLECTION

The structure factor depends upon the atomic positions and these were represented by the cell vectors  $\mathbf{r}_n$ . It is convenient to express the cell vectors in terms of components along  $\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3$  by means of fractional coordinates  $x_n, y_n, z_n$ , which are numbers between zero and unity. As illustrated by Fig. 3.3,  $\mathbf{r}_n = x_n\mathbf{a}_1 + y_n\mathbf{a}_2 + z_n\mathbf{a}_3$ . For an  $hkl$ -reflection, we are interested in the value of the structure factor when the Bragg law is satisfied for this set of planes, and hence when  $\mathbf{s} - \mathbf{s}_0 = \lambda\mathbf{H}_{hkl}$ . Expressing the cell vectors in terms of fractional coordinates, and using the  $(\mathbf{s} - \mathbf{s}_0)$  value which corresponds to an  $hkl$ -reflection, Eq. (3.2) becomes

$$F_{hkl} = \sum_n f_n e^{2\pi i(hb_1+kb_2+lb_3)\cdot(x_n\mathbf{a}_1+y_n\mathbf{a}_2+z_n\mathbf{a}_3)} = \sum_n f_n e^{2\pi i(hx_n+ky_n+lz_n)}. \quad (3.10)$$

**Fig. 3.3** Representation of the basis vector  $\mathbf{r}_n$  in terms of the fractional coordinates  $x_n$ ,  $y_n$ , and  $z_n$ .



In a crystal whose Bravais lattice is face-centered, for every atom with fractional coordinates  $x_n y_n z_n$ , there must be three identical atoms with coordinates  $x_n + \frac{1}{2}, y_n + \frac{1}{2}, z_n$ ;  $x_n + \frac{1}{2}, y_n, z_n + \frac{1}{2}$ ; and  $x_n, y_n + \frac{1}{2}, z_n + \frac{1}{2}$ . If the cell contains  $n$  atoms, there are  $n/4$  groups of four, all four atoms in each group having the same scattering factor. The structure factor can be expressed as a sum over such groups of 4 atoms:

$$F_{hkl} = \sum_{n/4} f_n \{ e^{2\pi i(hx_n + ky_n + lz_n)} + e^{2\pi i(h[x_n + 1/2] + k[y_n + 1/2] + lz_n)} \\ + e^{2\pi i(h[x_n + 1/2] + ky_n + l[z_n + 1/2])} + e^{2\pi i(hx_n + k[y_n + 1/2] + l[z_n + 1/2])} \}.$$

This can be written in the simpler form

$$F_{hkl} = [1 + e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)}] \sum_{n/4} f_n e^{2\pi i(hx_n + ky_n + lz_n)}. \quad (3.11)$$



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If  $m$  is an integer,  $e^{\pi im} = (-1)^m$ , and hence the first factor takes the value 4 if  $hkl$  are unmixed (all odd or all even) and the value zero if  $hkl$  are mixed:

$$hkl \text{ unmixed: } F_{hkl} = 4 \sum_{n/4} f_n e^{2\pi i(hx_n + ky_n + lz_n)}, \quad (3.12)$$

$$hkl \text{ mixed: } F_{hkl} = 0.$$

Regardless of the atomic coordinates  $x_n y_n z_n$ ,  $F_{hkl} = 0$  for all reflections with mixed  $hkl$ . Hence the face-centered Bravais lattice is recognized by the fact that all reflections with mixed indices are missing.

In a crystal whose Bravais lattice is body-centered, for every atom with fractional coordinates  $x_n y_n z_n$ , there must be an identical atom with coordinates  $x_n + \frac{1}{2}$ ,  $y_n + \frac{1}{2}$ , and  $z_n + \frac{1}{2}$ . The structure factor is expressed as a sum over such groups of 2 atoms:

$$F_{hkl} = [1 + e^{\pi i(h+k+l)}] \sum_{n/2} f_n e^{2\pi i(hx_n + ky_n + lz_n)}$$

and hence

$$h + k + l = \text{even}: \quad F_{hkl} = 2 \sum_{n/2} f_n e^{2\pi i(hx_n + ky_n + lz_n)}, \quad (3.13)$$

$$h + k + l = \text{odd}: \quad F_{hkl} = 0.$$

The body-centered Bravais lattice is recognized from the fact that all reflections will be missing for  $h + k + l = \text{odd}$ .

We next consider the evaluation of the structure factor for two common structures having the face-centered cubic Bravais lattice. In rock salt, the cubic cell contains 4 Na and 4 Cl at the following positions:

	0	0	0		$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
Cl	$\frac{1}{2}$	$\frac{1}{2}$	0	Na	0	0	$\frac{1}{2}$
	$\frac{1}{2}$	0	$\frac{1}{2}$		0	$\frac{1}{2}$	0
	0	$\frac{1}{2}$	$\frac{1}{2}$		$\frac{1}{2}$	0	0

To evaluate the structure factor using Eq. (3.12), we can choose any one of the positions in each group of 4 atoms. Using 0 0 0 for Cl and  $\frac{1}{2} \frac{1}{2} \frac{1}{2}$  for Na, the structure factor is given by

$$hkl \text{ mixed: } F_{hkl} = 0$$

$$hkl \text{ unmixed: } F_{hkl} = 4[f_{\text{Cl}} + f_{\text{Na}}e^{\pi i(h+k+l)}].$$

For rock salt, the structure factor takes the three forms:

$$hkl \text{ all even: } F_{hkl} = 4(f_{\text{Cl}} + f_{\text{Na}}),$$

$$hkl \text{ all odd: } F_{hkl} = 4(f_{\text{Cl}} - f_{\text{Na}}),$$

$$hkl \text{ mixed: } F_{hkl} = 0.$$

(3.14)