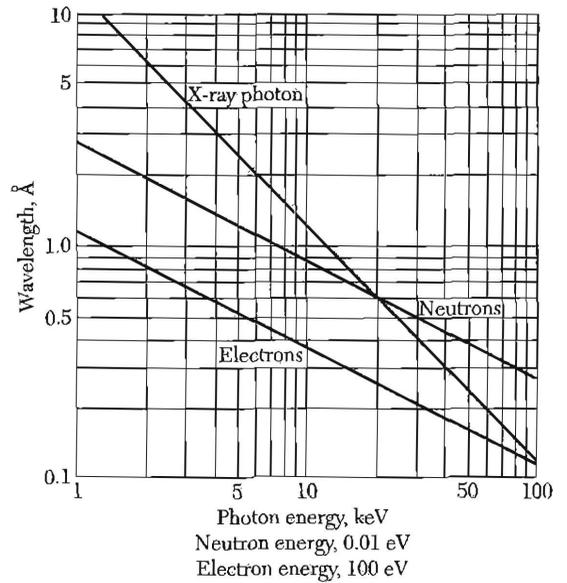


## 2

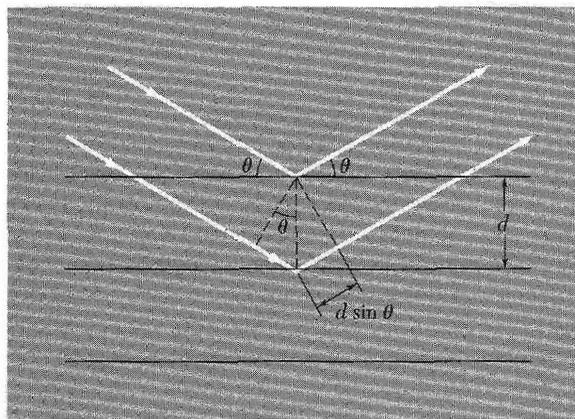
# *Wave Diffraction and the Reciprocal Lattice*

---

<b>DIFFRACTION OF WAVES BY CRYSTALS</b>	<b>25</b>
The Bragg law	25
<b>SCATTERED WAVE AMPLITUDE</b>	<b>26</b>
Fourier analysis	27
Reciprocal lattice vectors	29
Diffraction conditions	30
Laue equations	33
<b>BRILLOUIN ZONES</b>	<b>32</b>
Reciprocal lattice to sc lattice	34
Reciprocal lattice to bcc lattice	36
Reciprocal lattice to fcc lattice	37
<b>FOURIER ANALYSIS OF THE BASIS</b>	<b>39</b>
Structure factor of the bcc lattice	40
Structure factor of the fcc lattice	40
Atomic form factor	41
<b>SUMMARY</b>	<b>43</b>
<b>PROBLEMS</b>	<b>43</b>
1. Interplanar separation	43
2. Hexagonal space lattice	44
3. Volume of Brillouin zone	44
4. Width of diffraction maximum	44
5. Structure factor of diamond	45
6. Form factor of atomic hydrogen	45
7. Diatomic line	45



**Figure 1** Wavelength versus particle energy, for photons, neutrons, and electrons.



**Figure 2** Derivation of the Bragg equation  $2d \sin \theta = n\lambda$ ; here  $d$  is the spacing of parallel atomic planes and  $2\pi$  is the difference in phase between reflections from successive planes. The reflecting planes have nothing to do with the surface planes bounding the particular specimen.

## CHAPTER 2: WAVE DIFFRACTION AND THE RECIPROCAL LATTICE

### DIFFRACTION OF WAVES BY CRYSTALS

#### *The Bragg law*

We study crystal structure through the diffraction of photons, neutrons, and electrons (Fig. 1). The diffraction depends on the crystal structure and on the wavelength. At optical wavelengths such as 5000 Å, the superposition of the waves scattered elastically by the individual atoms of a crystal results in ordinary optical refraction. When the wavelength of the radiation is comparable with or smaller than the lattice constant, we may find diffracted beams in directions quite different from the incident direction.

W. L. Bragg presented a simple explanation of the diffracted beams from a crystal. The Bragg derivation is simple but is convincing only because it reproduces the correct result. Suppose that the incident waves are reflected specularly from parallel planes of atoms in the crystal, with each plane reflecting only a very small fraction of the radiation, like a lightly silvered mirror. In specular (mirrorlike) reflection the angle of incidence is equal to the angle of reflection. The diffracted beams are found when the reflections from parallel planes of atoms interfere constructively, as in Fig. 2. We treat elastic scattering, in which the energy of the x-ray is not changed on reflection.

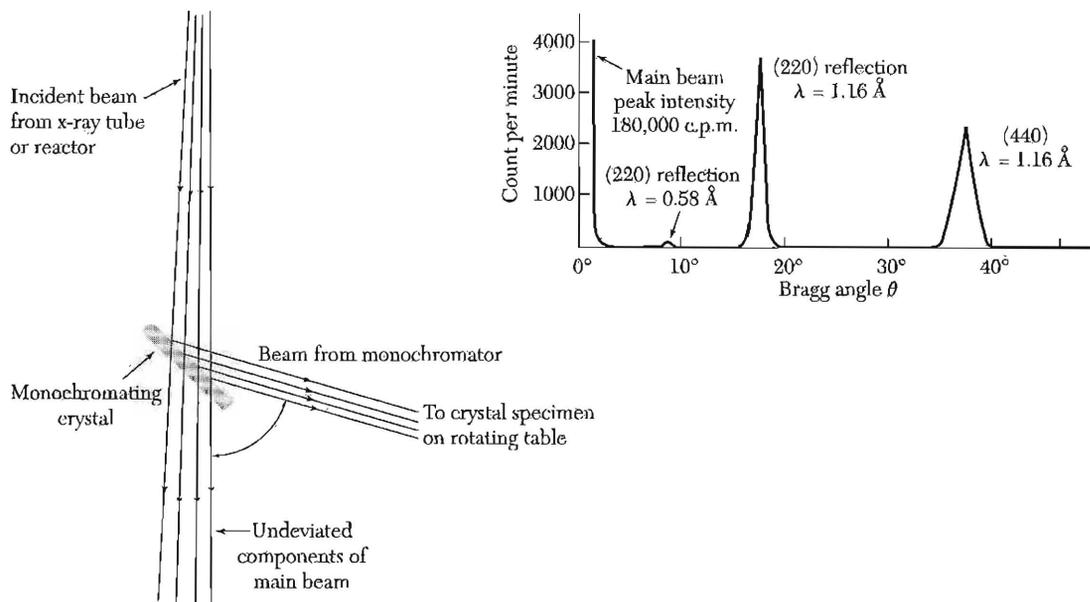
Consider parallel lattice planes spaced  $d$  apart. The radiation is incident in the plane of the paper. The path difference for rays reflected from adjacent planes is  $2d \sin \theta$ , where  $\theta$  is measured from the plane. Constructive interference of the radiation from successive planes occurs when the path difference is an integral number  $n$  of wavelengths  $\lambda$ , so that

$$2d \sin \theta = n\lambda \quad (1)$$

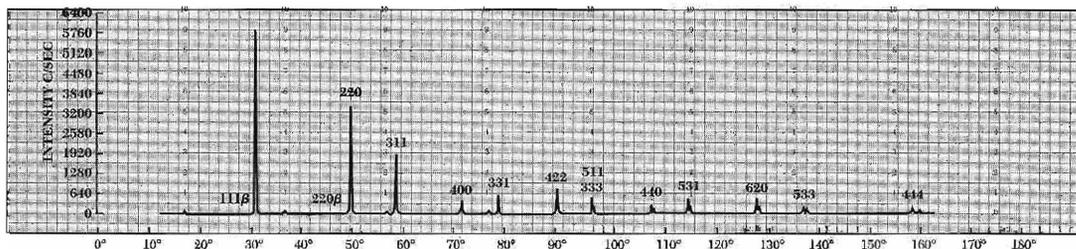
This is the Bragg law, which can be satisfied only for wavelength  $\lambda \leq 2d$ .

Although the reflection from each plane is specular, for only certain values of  $\theta$  will the reflections from all periodic parallel planes add up in phase to give a strong reflected beam. If each plane were perfectly reflecting, only the first plane of a parallel set would see the radiation, and any wavelength would be reflected. But each plane reflects  $10^{-3}$  to  $10^{-5}$  of the incident radiation, so that  $10^3$  to  $10^5$  planes may contribute to the formation of the Bragg-reflected beam in a perfect crystal. Reflection by a single plane of atoms is treated in Chapter 17 on surface physics.

The Bragg law is a consequence of the periodicity of the lattice. Notice that the law does not refer to the composition of the basis of atoms associated



**Figure 3** Sketch of a monochromator which by Bragg reflection selects a narrow spectrum of x-ray or neutron wavelengths from a broad spectrum incident beam. The upper part of the figure shows the analysis (obtained by reflection from a second crystal) of the purity of a 1.16 Å beam of neutrons from a calcium fluoride crystal monochromator. (After G. Bacon.)



**Figure 4** X-ray diffractometer recording of powdered silicon, showing a counter recording of the diffracted beams. (Courtesy of W. Parrish.)

with every lattice point. We shall see, however, that the composition of the basis determines the relative intensity of the various orders of diffraction (denoted by  $n$  above) from a given set of parallel planes. Bragg reflection from a single crystal is shown in Fig. 3 and from a powder in Fig. 4.

#### SCATTERED WAVE AMPLITUDE

The Bragg derivation of the diffraction condition (1) gives a neat statement of the condition for the constructive interference of waves scattered from the lattice points. We need a deeper analysis to determine the scattering

intensity from the basis of atoms, which means from the spatial distribution of electrons within each cell.

### Fourier Analysis

We have seen that a crystal is invariant under any translation of the form  $\mathbf{T} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3$ , where  $u_1, u_2, u_3$  are integers and  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  are the crystal axes. Any local physical property of the crystal, such as the charge concentration, electron number density, or magnetic moment density is invariant under  $\mathbf{T}$ . What is most important to us here is that the electron number density  $n(\mathbf{r})$  is a periodic function of  $\mathbf{r}$ , with periods  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  in the directions of the three crystal axes, respectively. Thus

$$n(\mathbf{r} + \mathbf{T}) = n(\mathbf{r}) . \quad (2)$$

Such periodicity creates an ideal situation for Fourier analysis. The most interesting properties of crystals are directly related to the Fourier components of the electron density.

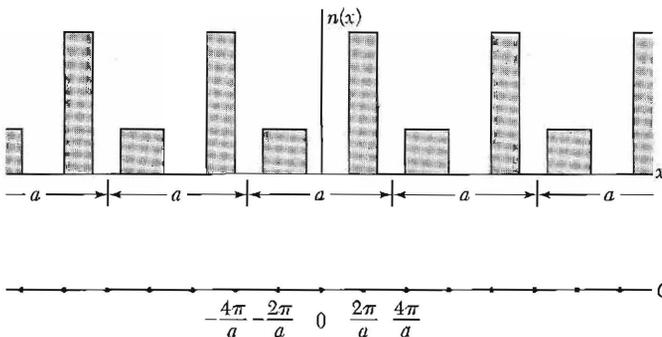
We consider first a function  $n(x)$  in one dimension with period  $a$  in the direction  $x$ . We expand  $n(x)$  in a Fourier series of sines and cosines:

$$n(x) = n_0 + \sum_{p>0} [C_p \cos(2\pi px/a) + S_p \sin(2\pi px/a)] , \quad (3)$$

where the  $p$  are positive integers and  $C_p, S_p$  are real constants, called the Fourier coefficients of the expansion. The factor  $2\pi/a$  in the arguments ensures that  $n(x)$  has the period  $a$ :

$$\begin{aligned} n(x+a) &= n_0 + \sum [C_p \cos(2\pi px/a + 2\pi p) + S_p \sin(2\pi px/a + 2\pi p)] \\ &= n_0 + \sum [C_p \cos(2\pi px/a) + S_p \sin(2\pi px/a)] = n(x) . \end{aligned} \quad (4)$$

We say that  $2\pi p/a$  is a point in the reciprocal lattice or Fourier space of the crystal. In one dimension these points lie on a line. The **reciprocal lattice points** tell us the allowed terms in the Fourier series (4) or (5). A term is allowed if it is consistent with the periodicity of the crystal, as in Fig. 5; other



**Figure 5**  
period  $a$ .  
may appear  
 $n(x) = \sum$

points in the reciprocal space are not allowed in the Fourier expansion of a periodic function.

It is convenient to write the series (4) in the compact form

$$n(x) = \sum_p n_p \exp(i2\pi px/a) , \quad (5)$$

where the sum is over all integers  $p$ : positive, negative, and zero. The coefficients  $n_p$  now are complex numbers. To ensure that  $n(x)$  is a real function, we require

$$n_{-p}^* = n_p , \quad (6)$$

for then the sum of the terms in  $p$  and  $-p$  is real. The asterisk on  $n_{-p}^*$  denotes the complex conjugate of  $n_{-p}$ .

With  $\varphi = 2\pi px/a$ , the sum of the terms in  $p$  and  $-p$  in (5) is real if (6) is satisfied. The sum is

$$\begin{aligned} n_p(\cos \varphi + i \sin \varphi) + n_{-p}(\cos \varphi - i \sin \varphi) \\ = (n_p + n_{-p})\cos \varphi + i(n_p - n_{-p})\sin \varphi , \end{aligned} \quad (7)$$

which in turn is equal to the real function

$$2\text{Re}\{n_p\} \cos \varphi - 2\text{Im}\{n_p\} \sin \varphi \quad (8)$$

if (6) is satisfied. Here  $\text{Re}\{n_p\}$  and  $\text{Im}\{n_p\}$  are real and denote the real and imaginary parts of  $n_p$ . Thus the number density  $n(x)$  is a real function, as desired.

The extension of the Fourier analysis to periodic functions  $n(\mathbf{r})$  in three dimensions is straightforward. We must find a set of vectors  $\mathbf{G}$  such that

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r}) \quad (9)$$

is invariant under all crystal translations  $\mathbf{T}$  that leave the crystal invariant. It will be shown below that the set of Fourier coefficients  $n_{\mathbf{G}}$  determines the x-ray scattering amplitude.

**Inversion of Fourier Series.** We now show that the Fourier coefficient  $n_p$  in the series (5) is given by

$$n_p = a^{-1} \int_0^a dx n(x) \exp(-i2\pi px/a) . \quad (10)$$

Substitute (5) in (10) to obtain

$$n_p = a^{-1} \sum_{p'} n_{p'} \int_0^a dx \exp[i2\pi(p' - p)x/a] . \quad (11)$$

If  $p' \neq p$  the value of the integral is

$$\frac{a}{i2\pi(p' - p)} (e^{i2\pi(p' - p)} - 1) = 0 ,$$

because  $p' - p$  is an integer and  $\exp[i2\pi(\text{integer})] = 1$ . For the term  $p' = p$  the integrand is  $\exp(i0) = 1$ , and the value of the integral is  $a$ , so that  $n_p = a^{-1}n_p a = n_p$ , which is an identity, so that (10) is an identity.

As in (10), the inversion of (9) gives

$$n_{\mathbf{G}} = V_c^{-1} \int_{\text{cell}} dV n(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) . \quad (12)$$

Here  $V_c$  is the volume of a cell of the crystal.

### Reciprocal Lattice Vectors

To proceed further with the Fourier analysis of the electron concentration we must find the vectors  $\mathbf{G}$  of the Fourier sum  $\sum n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r})$  as in (9). There is a powerful, somewhat abstract procedure for doing this. The procedure forms the theoretical basis for much of solid state physics, where Fourier analysis is the order of the day.

We construct the axis vectors  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  of the **reciprocal lattice**:

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} ; \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} ; \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} . \quad (13)$$

The factors  $2\pi$  are not used by crystallographers but are convenient in solid state physics.

If  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  are primitive vectors of the crystal lattice, then  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  are **primitive vectors of the reciprocal lattice**. Each vector defined by (13) is orthogonal to two axis vectors of the crystal lattice. Thus  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  have the property

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} , \quad (14)$$

where  $\delta_{ij} = 1$  if  $i = j$  and  $\delta_{ij} = 0$  if  $i \neq j$ .

Points in the reciprocal lattice are mapped by the set of vectors

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3 , \quad (15)$$

where  $v_1, v_2, v_3$  are integers. A vector  $\mathbf{G}$  of this form is a **reciprocal lattice vector**.

The vectors  $\mathbf{G}$  in the Fourier series (9) are just the reciprocal lattice vectors (15), for then the Fourier series representation of the electron density has the desired invariance under any crystal translation  $\mathbf{T} = u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3$ . From (9),

$$n(\mathbf{r} + \mathbf{T}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r}) \exp(i\mathbf{G} \cdot \mathbf{T}) . \quad (16)$$

But  $\exp(i\mathbf{G} \cdot \mathbf{T}) = 1$ , because

$$\begin{aligned} \exp(i\mathbf{G} \cdot \mathbf{T}) &= \exp[i(v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3) \cdot (u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3)] \\ &= \exp[i2\pi(v_1u_1 + v_2u_2 + v_3u_3)] . \end{aligned} \quad (17)$$

The argument of the exponential has the form  $2\pi i$  times an integer, because  $v_1u_1 + v_2u_2 + v_3u_3$  is an integer, being the sum of products of integers. Thus by (9) we have the desired invariance,  $n(\mathbf{r} + \mathbf{T}) = n(\mathbf{r}) = \sum n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r})$ .

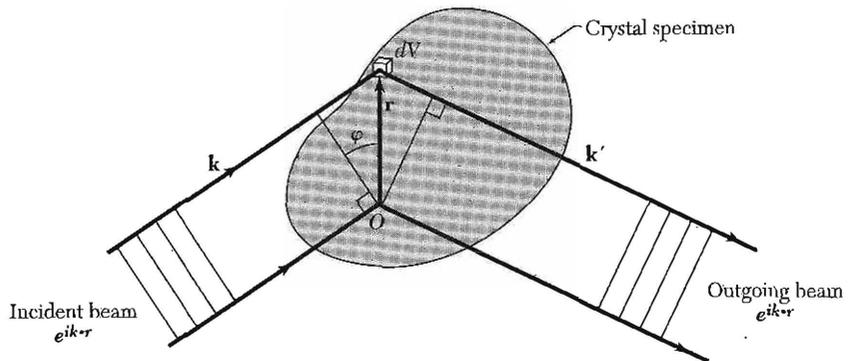
Every crystal structure has two lattices associated with it, the crystal lattice and the reciprocal lattice. A diffraction pattern of a crystal is, as we shall show, a map of the reciprocal lattice of the crystal. A microscope image, if it could be resolved on a fine enough scale, is a map of the crystal structure in real space. The two lattices are related by the definitions (13). Thus when we rotate a crystal in a holder, we rotate both the direct lattice and the reciprocal lattice.

Vectors in the direct lattice have the dimensions of [length]; vectors in the reciprocal lattice have the dimensions of [1/length]. The reciprocal lattice is a lattice in the Fourier space associated with the crystal. The term is motivated below. Wavevectors are always drawn in Fourier space, so that every position in Fourier space may have a meaning as a description of a wave, but there is a special significance to the points defined by the set of  $\mathbf{G}$ 's associated with a crystal structure.

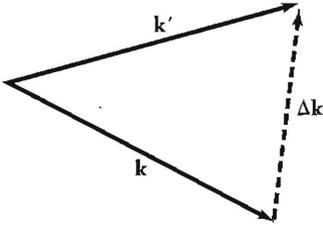
### Diffraction Conditions

**Theorem.** The set of reciprocal lattice vectors  $\mathbf{G}$  determines the possible x-ray reflections.

We see in Fig. 6 that the difference in phase factors is  $\exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}]$  between beams scattered from volume elements  $\mathbf{r}$  apart. The wavevectors of the incoming and outgoing beams are  $\mathbf{k}$  and  $\mathbf{k}'$ . We suppose that the amplitude



**Figure 6** The difference in path length of the incident wave  $\mathbf{k}$  at the points  $O$ ,  $\mathbf{r}$  is  $r \sin \phi$ , and the difference in phase angle is  $(2\pi r \sin \phi)/\lambda$ , which is equal to  $\mathbf{k} \cdot \mathbf{r}$ . For the diffracted wave the difference in phase angle is  $-\mathbf{k}' \cdot \mathbf{r}$ . The total difference in phase angle is  $(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}$ , and the wave scattered from  $dV$  at  $\mathbf{r}$  has the phase factor  $\exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}]$  relative to the wave scattered from a volume element at the origin  $O$ .



**Figure 7** Definition of the scattering vector  $\Delta\mathbf{k}$  such that  $\mathbf{k} + \Delta\mathbf{k} = \mathbf{k}'$ . In elastic scattering the magnitudes satisfy  $k' = k$ . Further, in Bragg scattering from a periodic lattice, any allowed  $\Delta\mathbf{k}$  must equal some reciprocal lattice vector  $\mathbf{G}$ .

of the wave scattered from a volume element is proportional to the local electron concentration  $n(\mathbf{r})$ . The total amplitude of the scattered wave in the direction of  $\mathbf{k}'$  is proportional to the integral over the crystal of  $n(\mathbf{r}) dV$  times the phase factor  $\exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}]$ .

In other words, the amplitude of the electric or magnetic field vectors in the scattered electromagnetic wave is proportional to the following integral which defines the quantity  $F$  that we call the **scattering amplitude**:

$$F = \int dV n(\mathbf{r}) \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}] = \int dV n(\mathbf{r}) \exp(-i\Delta\mathbf{k} \cdot \mathbf{r}) , \quad (18)$$

where  $\mathbf{k} - \mathbf{k}' = -\Delta\mathbf{k}$ , or

$$\mathbf{k} + \Delta\mathbf{k} = \mathbf{k}' . \quad (19)$$

Here  $\Delta\mathbf{k}$  measures the change in wavevector and is called the **scattering vector** (Fig. 7). We add  $\Delta\mathbf{k}$  to  $\mathbf{k}$  to obtain  $\mathbf{k}'$ , the wavevector of the scattered beam.

We introduce into (18) the Fourier components (9) of  $n(\mathbf{r})$  to obtain for the scattering amplitude

$$F = \sum_{\mathbf{G}} \int dV n_{\mathbf{G}} \exp[i(\mathbf{G} - \Delta\mathbf{k}) \cdot \mathbf{r}] . \quad (20)$$

When the scattering vector  $\Delta\mathbf{k}$  is equal to a particular reciprocal lattice vector,

$$\Delta\mathbf{k} = \mathbf{G} , \quad (21)$$

the argument of the exponential vanishes and  $F = Vn_{\mathbf{G}}$ . It is a simple exercise (Problem 4) to show that  $F$  is negligibly small when  $\Delta\mathbf{k}$  differs significantly from any reciprocal lattice vector.

In elastic scattering of a photon its energy  $\hbar\omega$  is conserved, so that the frequency  $\omega' = ck'$  of the emergent beam is equal to the frequency of the incident beam. Thus the magnitudes  $k$  and  $k'$  are equal, and  $k^2 = k'^2$ , a result that holds also for elastic scattering of electron and neutron beams. From (21) we found  $\Delta\mathbf{k} = \mathbf{G}$  or  $\mathbf{k} + \mathbf{G} = \mathbf{k}'$ , so that the **diffraction condition** is written as  $(\mathbf{k} + \mathbf{G})^2 = k^2$ , or

$$2\mathbf{k} \cdot \mathbf{G} + G^2 = 0 . \quad (22)$$

This is the central result of the theory of elastic scattering of waves in a periodic lattice. If  $\mathbf{G}$  is a reciprocal lattice vector, so is  $-\mathbf{G}$ , and with this substitution we can write (22) as

$$2\mathbf{k} \cdot \mathbf{G} = G^2 \quad (23)$$

This particular expression is often used as the condition for diffraction.

Equation (23) is another statement of the Bragg condition (1). The result of Problem 1 is that the spacing  $d(hkl)$  between parallel lattice planes that are normal to the direction  $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$  is  $d(hkl) = 2\pi/|\mathbf{G}|$ . Thus the result  $2\mathbf{k} \cdot \mathbf{G} = G^2$  may be written as

$$2(2\pi/\lambda) \sin \theta = 2\pi/d(hkl) \quad ,$$

or  $2d(hkl) \sin \theta = \lambda$ . Here  $\theta$  is the angle between the incident beam and the crystal plane.

The integers  $hkl$  that define  $\mathbf{G}$  are not necessarily identical with the indices of an actual crystal plane, because the  $hkl$  may contain a common factor  $n$ , whereas in the definition of the indices in Chapter 1 the common factor has been eliminated. We thus obtain the Bragg result:

$$2d \sin \theta = n\lambda \quad , \quad (24)$$

where  $d$  is the spacing between adjacent parallel planes with indices  $h/n$ ,  $k/n$ ,  $l/n$ .

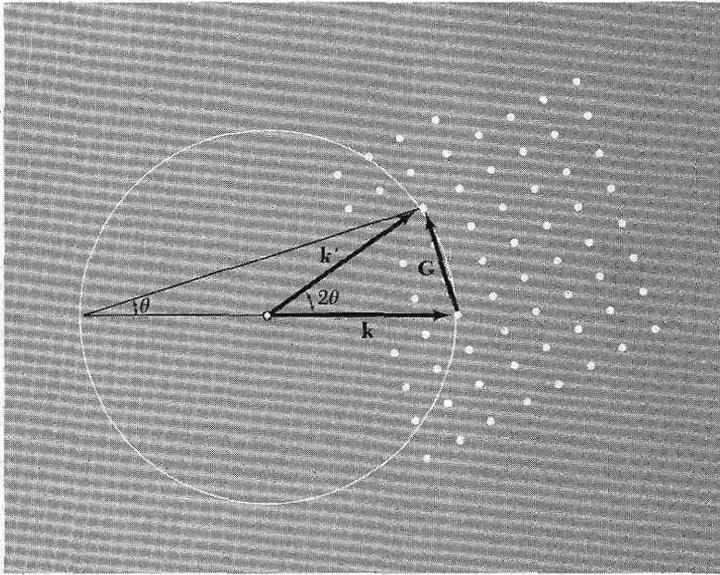
### Laue Equations

The original result (21) of diffraction theory, namely that  $\Delta\mathbf{k} = \mathbf{G}$ , may be expressed in another way to give what are called the Laue equations. These are valuable because of their geometrical representation. Take the scalar product of both  $\Delta\mathbf{k}$  and  $\mathbf{G}$  successively with  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ ,  $\mathbf{a}_3$ . From (14) and (15) we get

$$\mathbf{a}_1 \cdot \Delta\mathbf{k} = 2\pi v_1 \quad ; \quad \mathbf{a}_2 \cdot \Delta\mathbf{k} = 2\pi v_2 \quad ; \quad \mathbf{a}_3 \cdot \Delta\mathbf{k} = 2\pi v_3 \quad . \quad (25)$$

These equations have a simple geometrical interpretation. The first equation  $\mathbf{a}_1 \cdot \Delta\mathbf{k} = 2\pi v_1$  tells us that  $\Delta\mathbf{k}$  lies on a certain cone about the direction of  $\mathbf{a}_1$ . The second equation tells us that  $\Delta\mathbf{k}$  lies on a cone about  $\mathbf{a}_2$  as well, and the third equation requires that  $\Delta\mathbf{k}$  lies on a cone about  $\mathbf{a}_3$ . Thus, at a reflection  $\Delta\mathbf{k}$  must satisfy all three equations; it must lie at the common line of intersection of *three* cones, which is a severe condition that can be satisfied only by systematic sweeping or searching in wavelength or crystal orientation—or by sheer accident.

A beautiful construction, the Ewald construction, is exhibited in Fig. 8. This helps us visualize the nature of the accident that must occur in order to satisfy the diffraction condition in three dimensions.



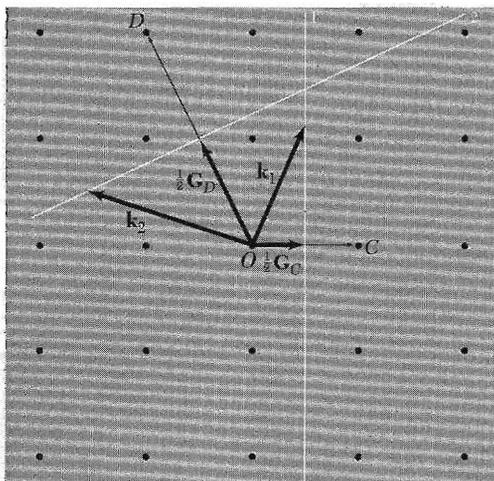
**Figure 8** The points on the right-hand side are reciprocal-lattice points of the crystal. The vector  $\mathbf{k}$  is drawn in the direction of the incident x-ray beam, and the origin is chosen such that  $\mathbf{k}$  terminates at any reciprocal lattice point. We draw a sphere of radius  $k = 2\pi/\lambda$  about the origin of  $\mathbf{k}$ . A diffracted beam will be formed if this sphere intersects any other point in the reciprocal lattice. The sphere as drawn intercepts a point connected with the end of  $\mathbf{k}$  by a reciprocal lattice vector  $\mathbf{G}$ . The diffracted x-ray beam is in the direction  $\mathbf{k}' = \mathbf{k} + \mathbf{G}$ . The angle  $\theta$  is the Bragg angle of Fig. 2. This construction is due to P. P. Ewald.

### BRILLOUIN ZONES

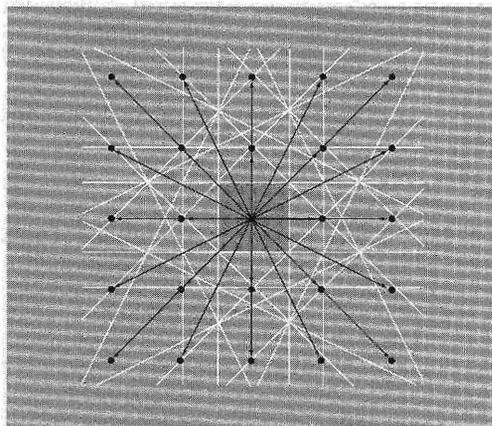
Brillouin gave the statement of the diffraction condition that is most widely used in solid state physics, which means in the description of electron energy band theory and of the elementary excitations of other kinds. A Brillouin zone is defined as a Wigner-Seitz primitive cell in the reciprocal lattice. (The construction in the direct lattice was shown in Fig. 1.4.) The Brillouin zone gives a vivid geometrical interpretation of the diffraction condition  $2\mathbf{k} \cdot \mathbf{G} = G^2$  of Eq. (23). We divide both sides by 4 to obtain

$$\mathbf{k} \cdot \left(\frac{1}{2}\mathbf{G}\right) = \left(\frac{1}{2}G\right)^2. \quad (26)$$

We now work in reciprocal space, the space of the  $\mathbf{k}$ 's and  $\mathbf{G}$ 's. Select a vector  $\mathbf{G}$  from the origin to a reciprocal lattice point. Construct a plane normal to this vector  $\mathbf{G}$  at its midpoint. This plane forms a part of a zone boundary (Fig. 9a). An x-ray beam in the crystal will be diffracted if its wavevector  $\mathbf{k}$  has the magnitude and direction required by (26). The diffracted beam will then be in the direction  $\mathbf{k} - \mathbf{G}$ , as we see from (19) with  $\Delta\mathbf{k} = -\mathbf{G}$ . Thus the Brillouin construction exhibits all the wavevectors  $\mathbf{k}$  which can be Bragg-reflected by the crystal.



**Figure 9a** Reciprocal lattice points near the point  $O$  at the origin of the reciprocal lattice. The reciprocal lattice vector  $\mathbf{G}_C$  connects points  $OC$ ; and  $\mathbf{G}_D$  connects  $OD$ . Two planes 1 and 2 are drawn which are the perpendicular bisectors of  $\mathbf{G}_C$  and  $\mathbf{G}_D$ , respectively. Any vector from the origin to the plane 1, such as  $\mathbf{k}_1$ , will satisfy the diffraction condition  $\mathbf{k}_1 \cdot (\frac{1}{2} \mathbf{G}_C) = (\frac{1}{2} \mathbf{G}_C)^2$ . Any vector from the origin to the plane 2, such as  $\mathbf{k}_2$ , will satisfy the diffraction condition  $\mathbf{k}_2 \cdot (\frac{1}{2} \mathbf{G}_D) = (\frac{1}{2} \mathbf{G}_D)^2$ .



**Figure 9b** Square reciprocal lattice with reciprocal lattice vectors shown as fine black lines. The lines shown in white are perpendicular bisectors of the reciprocal lattice vectors. The central square is the smallest volume about the origin which is bounded entirely by white lines. The square is the Wigner-Seitz primitive cell of the reciprocal lattice. It is called the first Brillouin zone.

The set of planes that are the perpendicular bisectors of the reciprocal lattice vectors is of general importance in the theory of wave propagation in crystals: A wave whose wavevector drawn from the origin terminates on any of these planes will satisfy the condition for diffraction. These planes divide the Fourier space of the crystal into fragments, as shown in Fig. 9b for a square lattice. The central square is a primitive cell of the reciprocal lattice. It is a Wigner-Seitz cell of the reciprocal lattice.

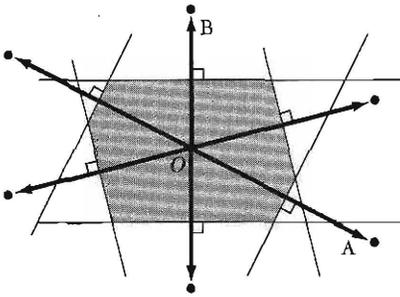
The central cell in the reciprocal lattice is of special importance in the theory of solids, and we call it the first Brillouin zone. *The first Brillouin zone is the smallest volume entirely enclosed by planes that are the perpendicular bisectors of the reciprocal lattice vectors drawn from the origin.* Examples are shown in Figs. 10 and 11.

Historically, Brillouin zones are not part of the language of x-ray diffraction analysis of crystal structures, but the zones are an essential part of the analysis of the electronic energy-band structure of crystals.

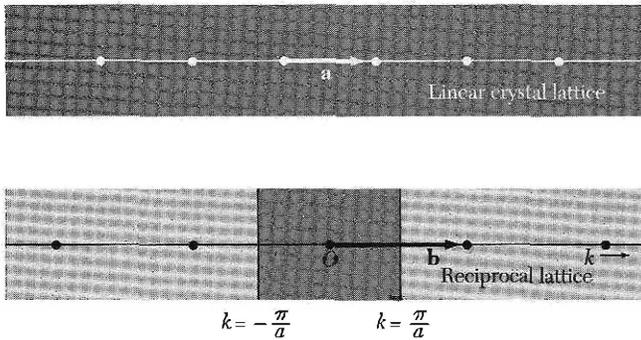
### **Reciprocal Lattice to sc Lattice**

The primitive translation vectors of a simple cubic lattice may be taken as the set

$$\mathbf{a}_1 = a\hat{x} ; \quad \mathbf{a}_2 = a\hat{y} ; \quad \mathbf{a}_3 = a\hat{z} . \quad (27a)$$



**Figure 10** Construction of the first Brillouin zone for an oblique lattice in two dimensions. We first draw a number of vectors from  $O$  to nearby points in the reciprocal lattice. Next we construct lines perpendicular to these vectors at their midpoints. The smallest enclosed area is the first Brillouin zone.

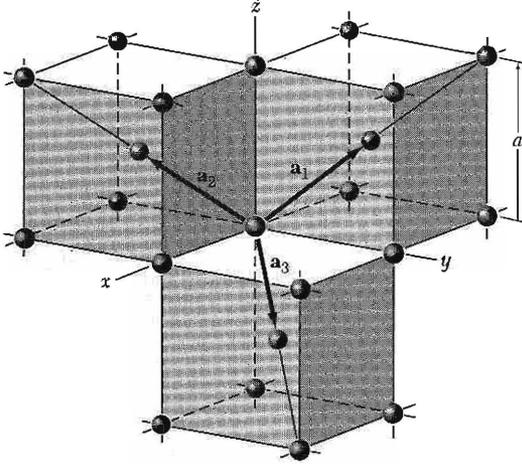


**Figure 11** Crystal and reciprocal lattices in one dimension. The basis vector in the reciprocal lattice is  $\mathbf{b}$ , of length equal to  $2\pi/a$ . The shortest reciprocal lattice vectors from the origin are  $\mathbf{b}$  and  $-\mathbf{b}$ . The perpendicular bisectors of these vectors form the boundaries of the first Brillouin zone. The boundaries are at  $k = \pm\pi/a$ .

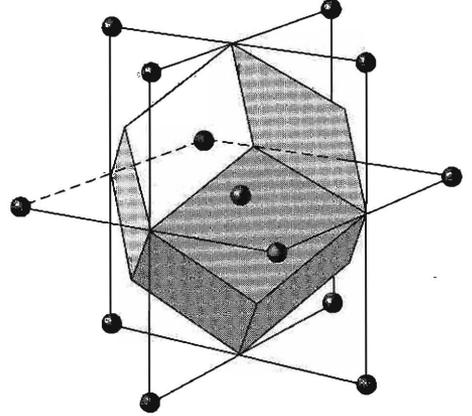
Here  $\hat{x}, \hat{y}, \hat{z}$  are orthogonal vectors of unit length. The volume of the cell is  $\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3 = a^3$ . The primitive translation vectors of the reciprocal lattice are found from the standard prescription (13):

$$\mathbf{b}_1 = (2\pi/a)\hat{x} ; \quad \mathbf{b}_2 = (2\pi/a)\hat{y} ; \quad \mathbf{b}_3 = (2\pi/a)\hat{z} . \quad (27b)$$

Here the reciprocal lattice is itself a simple cubic lattice, now of lattice constant  $2\pi/a$ .



**Figure 12** Primitive basis vectors of the body-centered cubic lattice.



**Figure 13** First Brillouin zone of the body-centered cubic lattice. The figure is a regular rhombic dodecahedron.

The boundaries of the first Brillouin zones are the planes normal to the six reciprocal lattice vectors  $\pm\mathbf{b}_1$ ,  $\pm\mathbf{b}_2$ ,  $\pm\mathbf{b}_3$  at their midpoints:

$$\pm\frac{1}{2}\mathbf{b}_1 = \pm(\pi/a)\hat{\mathbf{x}} ; \quad \pm\frac{1}{2}\mathbf{b}_2 = \pm(\pi/a)\hat{\mathbf{y}} ; \quad \pm\frac{1}{2}\mathbf{b}_3 = \pm(\pi/a)\hat{\mathbf{z}} . \quad (28)$$

The six planes bound a cube of edge  $2\pi/a$  and of volume  $(2\pi/a)^3$ ; this cube is the first Brillouin zone of the sc crystal lattice.

### ***Reciprocal Lattice to bcc Lattice***

The primitive translation vectors of the bcc lattice (Fig. 12) are

$$\mathbf{a}_1 = \frac{1}{2}a(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}) ; \quad \mathbf{a}_2 = \frac{1}{2}a(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}) ; \quad \mathbf{a}_3 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) , \quad (29)$$

where  $a$  is the side of the conventional cube and  $\hat{\mathbf{x}}$ ,  $\hat{\mathbf{y}}$ ,  $\hat{\mathbf{z}}$  are orthogonal unit vectors parallel to the cube edges. The volume of the primitive cell is

$$V = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| = \frac{1}{2}a^3 . \quad (30)$$

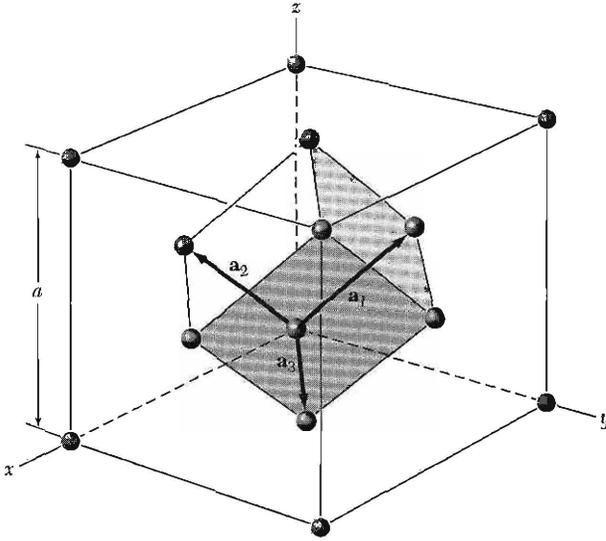
The primitive translations of the reciprocal lattice are defined by (13). We have, using (28),

$$\mathbf{b}_1 = (2\pi/a)(\hat{\mathbf{y}} + \hat{\mathbf{z}}) ; \quad \mathbf{b}_2 = (2\pi/a)(\hat{\mathbf{x}} + \hat{\mathbf{z}}) ; \quad \mathbf{b}_3 = (2\pi/a)(\hat{\mathbf{x}} + \hat{\mathbf{y}}) . \quad (31)$$

Note by comparison with Fig. 14 (p. 37) that these are just the primitive vectors of an fcc lattice, so that an fcc lattice is the reciprocal lattice of the bcc lattice.

The general reciprocal lattice vector is, for integral  $v_1, v_2, v_3$ ,

$$\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3 = (2\pi/a)[(v_2 + v_3)\hat{\mathbf{x}} + (v_1 + v_3)\hat{\mathbf{y}} + (v_1 + v_2)\hat{\mathbf{z}}] . \quad (32)$$



**Figure 14** Primitive basis vectors of the face-centered cubic lattice.

The shortest  $\mathbf{G}$ 's are the following 12 vectors, where all choices of sign are independent:

$$(2\pi/a)(\pm\hat{y} \pm \hat{z}) ; \quad (2\pi/a)(\pm\hat{x} \pm \hat{z}) ; \quad (2\pi/a)(\pm\hat{x} \pm \hat{y}) . \quad (33)$$

One primitive cell of the reciprocal lattice is the parallelepiped described by the  $\mathbf{b}_1$ ,  $\mathbf{b}_2$ ,  $\mathbf{b}_3$  defined by (31). The volume of this cell in reciprocal space is  $\mathbf{b}_1 \cdot \mathbf{b}_2 \times \mathbf{b}_3 = 2(2\pi/a)^3$ . The cell contains one reciprocal lattice point, because each of the eight corner points is shared among eight parallelepipeds. Each parallelepiped contains one-eighth of each of eight corner points (see Fig. 12).

Another primitive cell is the central (Wigner-Seitz) cell of the reciprocal lattice which is the first Brillouin zone. Each such cell contains one lattice point at the central point of the cell. This zone (for the bcc lattice) is bounded by the planes normal to the 12 vectors of Eq. (33) at their midpoints. The zone is a regular 12-faced solid, a rhombic dodecahedron, as shown in Fig. 13.

### **Reciprocal Lattice to fcc Lattice**

The primitive translation vectors of the fcc lattice of Fig. 14 are

$$\mathbf{a}_1 = \frac{1}{2}a(\hat{y} + \hat{z}) ; \quad \mathbf{a}_2 = \frac{1}{2}a(\hat{x} + \hat{z}) ; \quad \mathbf{a}_3 = \frac{1}{2}a(\hat{x} + \hat{y}) . \quad (34)$$

The volume of the primitive cell is

$$V = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| = \frac{1}{4}a^3 . \quad (35)$$



## FOURIER ANALYSIS OF THE BASIS

When the diffraction condition  $\Delta \mathbf{k} = \mathbf{G}$  of Eq. (21) is satisfied, the scattering amplitude (18) for a crystal of  $N$  cells may be written as

$$F_{\mathbf{G}} = N \int_{\text{cell}} dV n(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) = NS_{\mathbf{G}} . \quad (39)$$

The quantity  $S_{\mathbf{G}}$  is called the **structure factor** and is defined as an integral over a single cell, with  $\mathbf{r} = 0$  at one corner.

Often it is useful to write the electron concentration  $n(\mathbf{r})$  as the superposition of electron concentration functions  $n_j$  associated with each atom  $j$  of the cell. If  $\mathbf{r}_j$  is the vector to the center of atom  $j$ , then the function  $n_j(\mathbf{r} - \mathbf{r}_j)$  defines the contribution of that atom to the electron concentration at  $\mathbf{r}$ . The total electron concentration at  $\mathbf{r}$  due to all atoms in the single cell is the sum

$$n(\mathbf{r}) = \sum_{j=1}^s n_j(\mathbf{r} - \mathbf{r}_j) \quad (40)$$

over the  $s$  atoms of the basis. The decomposition of  $n(\mathbf{r})$  is not unique, for we cannot always say how much charge density is associated with each atom. This is not an important difficulty.

The structure factor defined by (39) may now be written as integrals over the  $s$  atoms of a cell:

$$\begin{aligned} S_{\mathbf{G}} &= \sum_j \int dV n_j(\mathbf{r} - \mathbf{r}_j) \exp(-i\mathbf{G} \cdot \mathbf{r}) \\ &= \sum_j \exp(-i\mathbf{G} \cdot \mathbf{r}_j) \int dV n_j(\boldsymbol{\rho}) \exp(-i\mathbf{G} \cdot \boldsymbol{\rho}) , \end{aligned} \quad (41)$$

where  $\boldsymbol{\rho} = \mathbf{r} - \mathbf{r}_j$ . We now define the **atomic form factor** as

$$f_j = \int dV n_j(\boldsymbol{\rho}) \exp(-i\mathbf{G} \cdot \boldsymbol{\rho}) , \quad (42)$$

integrated over all space. If  $n_j(\boldsymbol{\rho})$  is an atomic property,  $f_j$  is an atomic property.

We combine (41) and (42) to obtain the **structure factor of the basis** in the form

$$S_{\mathbf{G}} = \sum_j f_j \exp(-i\mathbf{G} \cdot \mathbf{r}_j) . \quad (43)$$

The usual form of this result follows on writing for atom  $j$ :

$$\mathbf{r}_j = x_j \mathbf{a}_1 + y_j \mathbf{a}_2 + z_j \mathbf{a}_3 , \quad (44)$$

as in (1.2). Then, for the reflection labelled by  $v_1, v_2, v_3$ , we have

$$\begin{aligned} \mathbf{G} \cdot \mathbf{r}_j &= (v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3) \cdot (x_j \mathbf{a}_1 + y_j \mathbf{a}_2 + z_j \mathbf{a}_3) \\ &= 2\pi(v_1 x_j + v_2 y_j + v_3 z_j) \quad , \end{aligned} \quad (45)$$

so that (43) becomes

$$S_{\mathbf{G}}(v_1 v_2 v_3) = \sum_j f_j \exp[-i2\pi(v_1 x_j + v_2 y_j + v_3 z_j)] \quad . \quad (46)$$

The structure factor  $S$  need not be real because the scattered intensity will involve  $S^*S$ , where  $S^*$  is the complex conjugate of  $S$  so that  $S^*S$  is real.

### **Structure Factor of the bcc Lattice**

The bcc basis referred to the cubic cell has identical atoms at  $x_1 = y_1 = z_1 = 0$  and at  $x_2 = y_2 = z_2 = \frac{1}{2}$ . Thus (46) becomes

$$S(v_1 v_2 v_3) = f[1 + \exp[-i\pi(v_1 + v_2 + v_3)]] \quad , \quad (47)$$

where  $f$  is the form factor of an atom. The value of  $S$  is zero whenever the exponential has the value  $-1$ , which is whenever the argument is  $-i\pi \times (\text{odd integer})$ . Thus we have

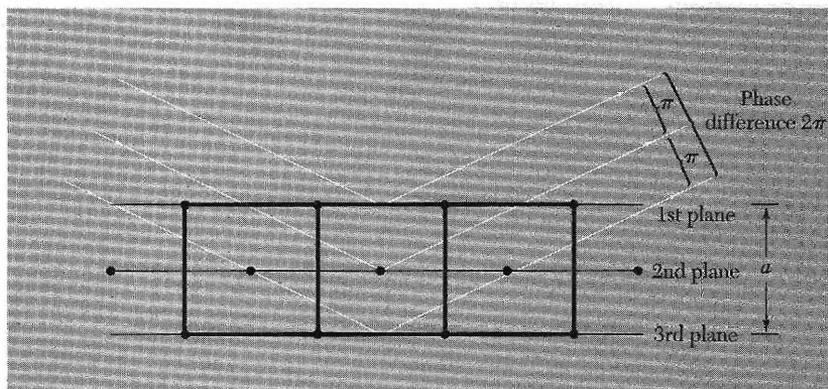
$$\begin{aligned} S &= 0 && \text{when } v_1 + v_2 + v_3 = \text{odd integer} \quad ; \\ S &= 2f && \text{when } v_1 + v_2 + v_3 = \text{even integer} \quad . \end{aligned}$$

Metallic sodium has a bcc structure. The diffraction pattern does not contain lines such as (100), (300), (111), or (221), but lines such as (200), (110), and (222) will be present; here the indices  $(v_1 v_2 v_3)$  are referred to a cubic cell. What is the physical interpretation of the result that the (100) reflection vanishes? The (100) reflection normally occurs when reflections from the planes that bound the cubic cell differ in phase by  $2\pi$ . In the bcc lattice there is an intervening plane (Fig. 16) of atoms, labeled the second plane in the figure, which is equal in scattering power to the other planes. Situated midway between them, it gives a reflection retarded in phase by  $\pi$  with respect to the first plane, thereby canceling the contribution from that plane. The cancellation of the (100) reflection occurs in the bcc lattice because the planes are identical in composition. A similar cancellation can easily be found in the hcp structure.

### **Structure Factor of the fcc Lattice**

The basis of the fcc structure referred to the cubic cell has identical atoms at  $000$ ;  $0\frac{1}{2}\frac{1}{2}$ ;  $\frac{1}{2}0\frac{1}{2}$ ;  $\frac{1}{2}\frac{1}{2}0$ . Thus (46) becomes

$$\begin{aligned} S(v_1 v_2 v_3) &= f[1 + \exp[-i\pi(v_2 + v_3)] + \exp[-i\pi(v_1 + v_3)] \\ &\quad + \exp[-i\pi(v_1 + v_2)]] \quad . \end{aligned} \quad (48)$$



**Figure 16** Explanation of the absence of a (100) reflection from a body-centered cubic lattice. The phase difference between successive planes is  $\pi$ , so that the reflected amplitude from two adjacent planes is  $1 + e^{-i\pi} = 1 - 1 = 0$ .

If all indices are even integers,  $S = 4f$ ; similarly if all indices are odd integers. But if only one of the integers is even, two of the exponents will be odd multiples of  $-i\pi$  and  $S$  will vanish. If only one of the integers is odd, the same argument applies and  $S$  will also vanish. Thus in the fcc lattice no reflections can occur for which the indices are partly even and partly odd.

The point is beautifully illustrated by Fig. 17: both KCl and KBr have an fcc lattice, but  $n(\mathbf{r})$  for KCl simulates an sc lattice because the  $\text{K}^+$  and  $\text{Cl}^-$  ions have equal numbers of electrons.

### Atomic Form Factor

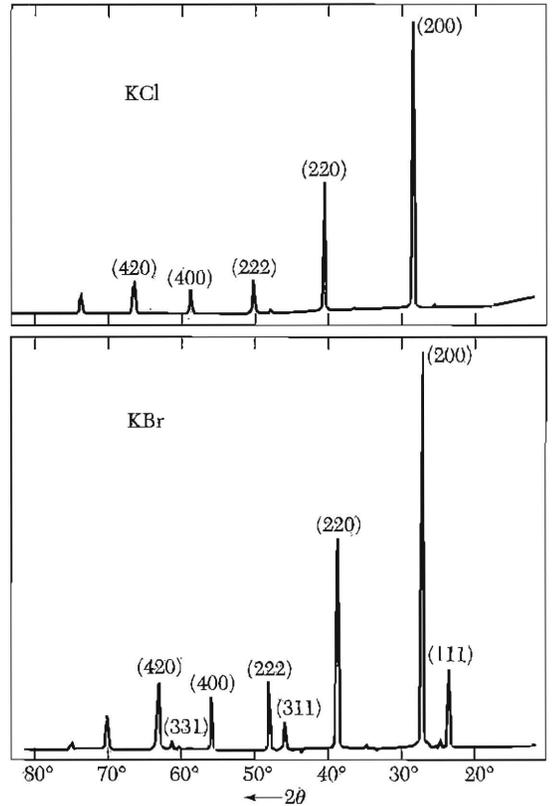
In the expression (46) for the structure factor, there occurs the quantity  $f_j$ , which is a measure of the scattering power of the  $j$ th atom in the unit cell. The value of  $f$  involves the number and distribution of atomic electrons, and the wavelength and angle of scattering of the radiation. We now give a classical calculation of the scattering factor.

The scattered radiation from a single atom takes account of interference effects within the atom. We defined the form factor in (42):

$$f_j = \int dV n_j(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) , \quad (49)$$

with the integral extended over the electron concentration associated with a single atom. Let  $\mathbf{r}$  make an angle  $\alpha$  with  $\mathbf{G}$ ; then  $\mathbf{G} \cdot \mathbf{r} = Gr \cos \alpha$ . If the electron distribution is spherically symmetric about the origin, then

$$\begin{aligned} f_j &\equiv 2\pi \int dr r^2 d(\cos \alpha) n_j(r) \exp(-iGr \cos \alpha) \\ &= 2\pi \int dr r^2 n_j(r) \cdot \frac{e^{iGr} - e^{-iGr}}{iGr} , \end{aligned}$$



**Figure 17** Comparison of x-ray reflections from KCl and KBr powders. In KCl the numbers of electrons of  $K^+$  and  $Cl^-$  ions are equal. The scattering amplitudes  $f(K^+)$  and  $f(Cl^-)$  are almost exactly equal, so that the crystal looks to x-rays as if it were a monatomic simple cubic lattice of lattice constant  $a/2$ . Only even integers occur in the reflection indices when these are based on a cubic lattice of lattice constant  $a$ . In KBr the form factor of  $Br^-$  is quite different to that of  $K^+$ , and all reflections of the fcc lattice are present. (Courtesy of R. van Nördstrand.)

after integration over  $d(\cos \alpha)$  between  $-1$  and  $1$ . Thus the form factor is given by

$$f_j = 4\pi \int dr n_j(r) r^2 = \frac{\sin Gr}{Gr} \quad (50)$$

If the same total electron density were concentrated at  $r = 0$ , only  $Gr = 0$  would contribute to the integrand. In this limit  $(\sin Gr)/Gr = 1$ , and

$$f_j = 4\pi \int dr n_j(r) r^2 = Z, \quad (51)$$

the number of atomic electrons. Therefore  $f$  is the ratio of the radiation amplitude scattered by the actual electron distribution in an atom to that scattered by one electron localized at a point. In the forward direction  $G = 0$ , and  $f$  reduces again to the value  $Z$ .

The overall electron distribution in a solid as seen in x-ray diffraction is fairly close to that of the appropriate free atoms. This statement does not mean that the outermost or valence electrons are not redistributed somewhat in forming the solid; it means only that the x-ray reflection intensities are represented well by the free atom values of the form factors and are not very sensitive to small redistributions of the electrons.

## SUMMARY

- Various statements of the Bragg condition:

$$2d \sin \theta = n\lambda ; \quad \Delta \mathbf{k} = \mathbf{G} ; \quad 2\mathbf{k} \cdot \mathbf{G} = G^2 .$$

- Laue conditions:

$$\mathbf{a}_1 \cdot \Delta \mathbf{k} = 2\pi v_1 ; \quad \mathbf{a}_2 \cdot \Delta \mathbf{k} = 2\pi v_2 ; \quad \mathbf{a}_3 \cdot \Delta \mathbf{k} = 2\pi v_3 .$$

- The primitive translation vectors of the reciprocal lattice are

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} ; \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} ; \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} .$$

Here  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  are the primitive translation vectors of the crystal lattice.

- A reciprocal lattice vector has the form

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3 ,$$

where  $v_1, v_2, v_3$  are integers or zero.

- The scattered amplitude in the direction  $\mathbf{k}' = \mathbf{k} + \Delta \mathbf{k} = \mathbf{k} + \mathbf{G}$  is proportional to the geometrical structure factor:

$$S_{\mathbf{G}} \equiv \sum f_j \exp(-i\mathbf{r}_j \cdot \mathbf{G}) = \sum f_j \exp[-i2\pi(x_j v_1 + y_j v_2 + z_j v_3)] ,$$

where  $j$  runs over the  $s$  atoms of the basis, and  $f_j$  is the atomic form factor (49) of the  $j$ th atom of the basis. The expression on the right-hand side is written for a reflection  $(v_1 v_2 v_3)$ , for which  $\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3$ .

- Any function invariant under a lattice translation  $\mathbf{T}$  may be expanded in a Fourier series of the form

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r}) .$$

- The first Brillouin zone is the Wigner-Seitz primitive cell of the reciprocal lattice. Only waves whose wavevector  $\mathbf{k}$  drawn from the origin terminates on a surface of the Brillouin zone can be diffracted by the crystal.

- |                          |                                |
|--------------------------|--------------------------------|
| • <i>Crystal lattice</i> | <i>First Brillouin zone</i>    |
| Simple cubic             | Cube                           |
| Body-centered cubic      | Rhombic dodecahedron (Fig. 13) |
| Face-centered cubic      | Truncated octahedron (Fig. 15) |

## Problems

1. **Interplanar separation.** Consider a plane  $hkl$  in a crystal lattice. (a) Prove that the reciprocal lattice vector  $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$  is perpendicular to this plane. (b) Prove that the distance between two adjacent parallel planes of the lattice is  $d(hkl) = 2\pi/|\mathbf{G}|$ . (c) Show for a simple cubic lattice that  $d^2 = a^2/(h^2 + k^2 + l^2)$ .

2. **Hexagonal space lattice.** The primitive translation vectors of the hexagonal space lattice may be taken as

$$\mathbf{a}_1 = (3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} ; \quad \mathbf{a}_2 = -(3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} ; \quad \mathbf{a}_3 = c\hat{\mathbf{z}} .$$

- (a) Show that the volume of the primitive cell is  $(3^{1/2}/2)a^2c$ .  
 (b) Show that the primitive translations of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} ; \quad \mathbf{b}_2 = -(2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} ; \quad \mathbf{b}_3 = (2\pi/c)\hat{\mathbf{z}} ,$$

so that the lattice is its own reciprocal, but with a rotation of axes.

- (c) Describe and sketch the first Brillouin zone of the hexagonal space lattice.

3. **Volume of Brillouin zone.** Show that the volume of the first Brillouin zone is  $(2\pi)^3/V_c$ , where  $V_c$  is the volume of a crystal primitive cell. Hint: The volume of a Brillouin zone is equal to the volume of the primitive parallelepiped in Fourier space. Recall the vector identity  $(\mathbf{c} \times \mathbf{a}) \times (\mathbf{a} \times \mathbf{b}) = (\mathbf{c} \cdot \mathbf{a} \times \mathbf{b})\mathbf{a}$ .

4. **Width of diffraction maximum.** We suppose that in a linear crystal there are identical point scattering centers at every lattice point  $\rho_m = m\mathbf{a}$ , where  $m$  is an integer. By analogy with (20), the total scattered radiation amplitude will be proportional to  $F = \sum \exp[-i m \mathbf{a} \cdot \Delta \mathbf{k}]$ . The sum over  $M$  lattice points is

$$F = \frac{1 - \exp[-iM(\mathbf{a} \cdot \Delta \mathbf{k})]}{1 - \exp[-i(\mathbf{a} \cdot \Delta \mathbf{k})]} ,$$

by the use of the series

$$\sum_{m=0}^{M-1} x^m = \frac{1 - x^M}{1 - x} .$$

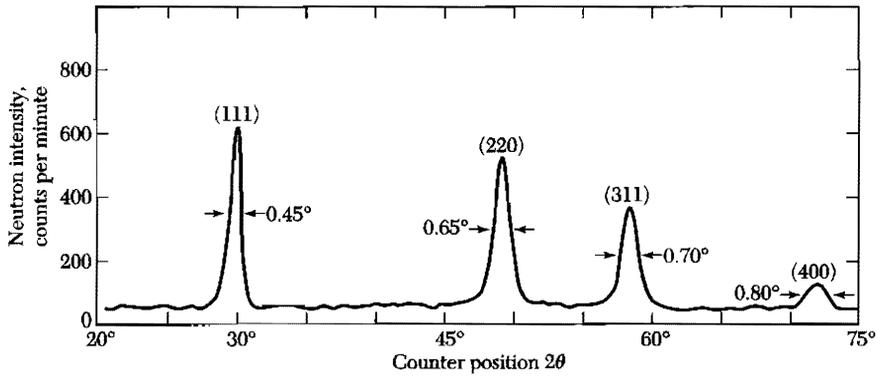
- (a) The scattered intensity is proportional to  $|F|^2$ . Show that

$$|F|^2 \equiv F \cdot F = \frac{\sin^2 \frac{1}{2} M(\mathbf{a} \cdot \Delta \mathbf{k})}{\sin^2 \frac{1}{2} (\mathbf{a} \cdot \Delta \mathbf{k})} .$$

- (b) We know that a diffraction maximum appears when  $\mathbf{a} \cdot \Delta \mathbf{k} = 2\pi h$ , where  $h$  is an integer. We change  $\Delta \mathbf{k}$  slightly and define  $\epsilon$  in  $\mathbf{a} \cdot \Delta \mathbf{k} = 2\pi h + \epsilon$  such that  $\epsilon$  gives the position of the first zero in  $\sin \frac{1}{2} M(\mathbf{a} \cdot \Delta \mathbf{k})$ . Show that  $\epsilon = 2\pi/M$ , so that the width of the diffraction maximum is proportional to  $1/M$  and can be extremely narrow for macroscopic values of  $M$ . The same result holds true for a three-dimensional crystal.

5. **Structure factor of diamond.** The crystal structure of diamond is described in Chapter 1. The basis consists of eight atoms if the cell is taken as the conventional cube. (a) Find the structure factor  $S$  of this basis. (b) Find the zeros of  $S$  and show that the allowed reflections of the diamond structure satisfy  $v_1 + v_2 + v_3 = 4n$ , where all indices are even and  $n$  is any integer, or else all indices are odd (Fig. 18). (Notice that  $h, k, l$  may be written for  $v_1, v_2, v_3$  and this is often done.)

6. **Form factor of atomic hydrogen.** For the hydrogen atom in its ground state, the number density is  $n(r) = (\pi a_0^3)^{-1} \exp(-2r/a_0)$ , where  $a_0$  is the Bohr radius. Show that the form factor is  $f_G = 16/(4 + G^2 a_0^2)^2$ .



**Figure 18** Neutron diffraction pattern for powdered diamond. (After G. Bacon.)

7. **Diatomic line.** Consider a line of atoms  $ABAB \dots AB$ , with an  $A-B$  bond length of  $\frac{1}{2}a$ . The form factors are  $f_A, f_B$  for atoms  $A, B$ , respectively. The incident beam of x-rays is perpendicular to the line of atoms. (a) Show that the interference condition is  $n\lambda = a \cos \theta$ , where  $\theta$  is the angle between the diffracted beam and the line of atoms. (b) Show that the intensity of the diffracted beam is proportional to  $|f_A - f_B|^2$  for  $n$  odd, and to  $|f_A + f_B|^2$  for  $n$  even. (c) Explain what happens if  $f_A = f_B$ .