

Section 2: X-ray Diffraction and Reciprocal Lattice

Bragg law. Most methods for determining the atomic structure of crystals are based of the idea of scattering of radiation. X-rays is one of the types of the radiation which can be used. The wavelength of the radiation should have a wavelength comparable to a typical interatomic distance which is in solids of a few angstroms (10^{-8} cm). The x-ray wavelength λ can be estimated as follows

$$E = h\nu = \frac{hc}{\lambda} \Rightarrow \lambda(\text{\AA}) = \frac{12.4}{E(\text{keV})}. \quad (2.1)$$

Therefore, x-rays of energy 2-10 keV are suitable for studying the crystal structure.

X-rays interact with electronic shells of atoms in a solid. Electrons absorb and re-radiate x-rays which can then be detected. Nuclei are too heavy to respond. The reflectivity of x-rays is of the order of 10^{-3} - 10^{-5} , so that the penetration in the solid is deep. Therefore, x-rays serve as a *bulk* probe.

In 1913 Bragg found that crystalline solids have remarkably characteristic patterns of reflected x-ray radiation. In crystalline materials, for certain wavelengths and incident directions, intense peaks of scattered radiation were observed. Bragg accounted for this by regarding a crystal as made out of parallel planes of atoms, spaced by distance d apart. The conditions for a sharp peak in the intensity of the scattered radiation were that:

- (1) the x-rays should be specularly reflected by the atoms in one plane;
- (2) the reflected rays from the successive planes interfere constructively.

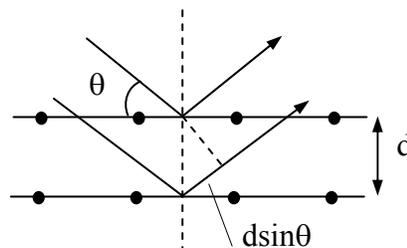


Fig.1

Fig.1 shows x-rays which are specularly reflected from adjacent planes. The path difference between the two x-rays is equal to $2d\sin\theta$. For the x-rays to interfere constructively this difference must be an integer number of wavelengths. This leads to the Bragg condition:

$$2d\sin\theta = m\lambda \quad (2.2)$$

The integer m is known as the *order* of the corresponding reflection (or order of interference).

There are a number of various setups for studying crystal structure using x-ray diffraction. In most cases, the wavelength of radiation is fixed, and the angle is varied to observe diffraction peaks corresponding to reflections from different crystallographic planes. Using the Bragg law one can then determine the distance between the planes.

The Bragg law is greatly oversimplified (but it works!). It

- (i) says nothing about intensity and width of x-ray diffraction peaks;
- (ii) neglects differences in scattering from different atoms;
- (iii) neglects distribution of charge around atoms.

Diffraction condition and reciprocal lattice. Later von Layer introduced a different approach for x-ray diffraction. He regarded a crystal as composed of identical atoms placed at the lattice sites \mathbf{T} and assumed that each atom can reradiate the incident radiation in all directions. Sharp peaks are observed only in the directions and at wavelengths for which the x-rays scattered from all lattice points interfere constructively.

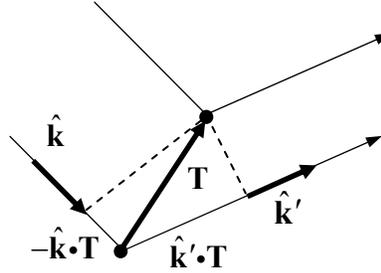


Fig.2

To find the condition of constructive interference we consider two scatterers (Fig.2) separated by a lattice vector \mathbf{T} . Let x-rays are incident from infinity, along direction $\hat{\mathbf{k}}$ with wavelength λ and wavevector $\mathbf{k} = 2\pi\hat{\mathbf{k}}/\lambda$. We assume that the scattering is *elastic*, i.e. the x-rays are scattered in $\hat{\mathbf{k}}'$ direction with *same* wavelength λ , so that the wavevector $\mathbf{k}' = 2\pi\hat{\mathbf{k}}'/\lambda$. The path difference between the x-ray scattered from the two atoms should be an integer number of wavelengths. Therefore, as is seen from Fig.2, the condition of constructive interference is

$$(\hat{\mathbf{k}}' - \hat{\mathbf{k}}) \cdot \mathbf{T} = m\lambda, \quad (2.3)$$

where m is an integer. Multiplying both sides of Eq.(2.3) by $2\pi/\lambda$ leads to a condition on the incident and scattered wave vectors:

$$(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{T} = 2\pi m. \quad (2.4)$$

Defining the *scattering wave vector* $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k}$, the diffraction condition can be written as

$$\Delta\mathbf{k} = \mathbf{G}, \quad (2.5)$$

where \mathbf{G} is, by definition, such a vector for which

$$\mathbf{G} \cdot \mathbf{T} = 2\pi m. \quad (2.6)$$

A set of vectors \mathbf{G} which satisfies this condition form a *reciprocal lattice*. Vectors \mathbf{G} are called *reciprocal lattice vectors*.

A reciprocal lattice is defined with reference to a particular Bravais lattice which is determined by a set of lattice vectors \mathbf{T} . The Bravais lattice that determines a particular reciprocal lattice is referred as the *direct lattice*, when viewed in relation to its reciprocal.

There is an algorithm for constructing the reciprocal lattice from the direct lattice. Let \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 be a set of primitive vectors of the direct lattice. Then the reciprocal lattice can be generated using primitive vectors

$$\mathbf{b}_1 = \frac{2\pi}{V} \mathbf{a}_2 \times \mathbf{a}_3, \quad \mathbf{b}_2 = \frac{2\pi}{V} \mathbf{a}_3 \times \mathbf{a}_1, \quad \mathbf{b}_3 = \frac{2\pi}{V} \mathbf{a}_1 \times \mathbf{a}_2, \quad (2.7)$$

where $V = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ is the volume of the unit cell, so that

$$\mathbf{G} = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3 \quad (2.8)$$

In order to prove that the vectors built in this way satisfy condition (2.6), we first note that the \mathbf{b}_i satisfy the condition

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} \quad (i,j=1,2,3) \quad (2.9)$$

where δ_{ij} is the Kronecker symbol defined by

$$\delta_{ij}=0, \text{ if } i \neq j \quad (2.10)$$

$$\delta_{ij}=1, \text{ if } i=j.$$

Indeed, since $\mathbf{T} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$, we obtain

$$\mathbf{G} \cdot \mathbf{T} = 2\pi(n_1 m_1 + n_2 m_2 + n_3 m_3), \quad (2.11)$$

which proves Eq.(2.6).

Examples: reciprocal lattices for 1D and 2D-rectangular structures. Note: Eqs.(2.9) rather than Eqs.(2.7) should be used in 1D and 2D cases.

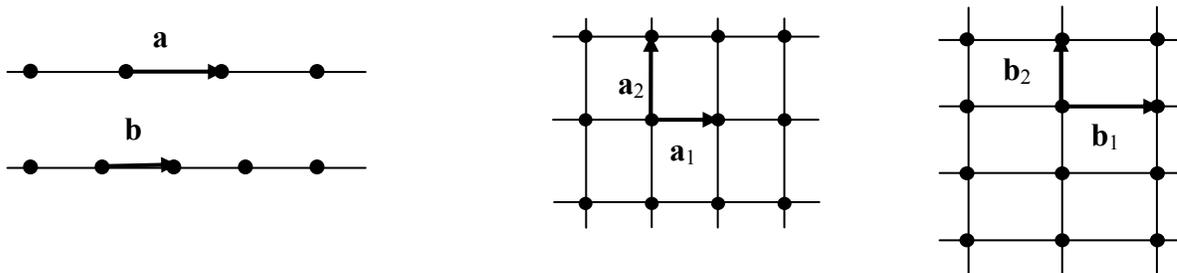


Fig.3 1D 2D

Reciprocal lattice types for some 3D lattices:

Direct lattice	Reciprocal lattice
sc	sc
bcc	fcc
fcc	bcc
hcp	hcp

Coming back to the diffraction condition (2.5), we can say that constructive interference occurs provided that the scattering wave vector is a vector of the reciprocal lattice.

It is sometimes more convenient to give a different formulation of the diffraction condition. In elastic scattering the photon energy is conserved, so that the magnitudes of k and k' are equal, and therefore $k^2 = k'^2$. Therefore, it follows from Eq.(2.5) that

$$\mathbf{k}'^2 = (\mathbf{G} + \mathbf{k})^2 \Rightarrow 0 = G^2 + 2\mathbf{k} \cdot \mathbf{G} \quad (2.12)$$

By replacing \mathbf{G} to $-\mathbf{G}$, which is also a reciprocal lattice vector, we arrive at

$$2\mathbf{k} \cdot \mathbf{G} = G^2, \quad (2.13)$$

that can be considered as the diffraction condition.

Equation (2.13) is another statement for the Bragg law (1). We prove this in three steps.

(1) We show that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is orthogonal to the plane represented by Miller indices (hkl) .

Consider the plane (hkl) which intercepts axes at points x, y , and z given in units a_1, a_2 and a_3 :

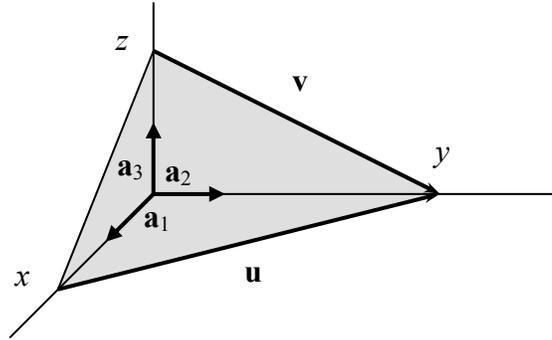


Fig.4

By the definition of the Miller indices we can always find such interceptions that

$$(h, k, l) = \left(\frac{1}{x}, \frac{1}{y}, \frac{1}{z} \right). \quad (2.14)$$

As we know, any plane can be defined by two non-collinear vectors lying within this plane. We can choose vectors \mathbf{u} and \mathbf{v} shown in Fig.4. They are given by $\mathbf{u} = y\mathbf{a}_2 - x\mathbf{a}_1$ and $\mathbf{v} = y\mathbf{a}_2 - z\mathbf{a}_3$. To prove that the reciprocal vector \mathbf{G} is normal to the plane (hkl) , it is sufficient to prove that this vector is orthogonal to \mathbf{u} and \mathbf{v} , i.e. $\mathbf{u} \cdot \mathbf{G} = 0$ and $\mathbf{v} \cdot \mathbf{G} = 0$. We have

$$\mathbf{u} \cdot \mathbf{G} = (y\mathbf{a}_2 - x\mathbf{a}_1) \cdot (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) = 2\pi(yk - xh) = 0, \quad (2.15)$$

where the second equation follows from the orthogonality condition of the vectors of the direct and reciprocal lattices (2.9) and the last equation follows from Eq.(2.14). In the same manner we can show that \mathbf{G} is orthogonal to \mathbf{v} . We have proved, therefore, that vector \mathbf{G} is orthogonal to the plane (hkl) .

(2) Now we prove that the distance between two adjacent parallel planes of the direct lattice is $d=2\pi/G$.

First, we note that the nearest plane which is parallel to the plane (hkl) goes through the origin of the Cartesian coordinates in Fig.4. Therefore, the interplanar distance is given by the projection of the one of the vectors $x\mathbf{a}_1, y\mathbf{a}_2, z\mathbf{a}_3$, to the direction normal to the (hkl) plane. This direction is given by the unit vector \mathbf{G}/G , since we have already established the \mathbf{G} is normal to the plane. Therefore

$$d = x\mathbf{a}_1 \cdot \mathbf{G} / G = 2\pi xh / G = 2\pi / G. \quad (2.16)$$

The connection between reciprocal vectors and crystal planes is now clear. The reciprocal vector $\mathbf{G}(hkl)$ is associated with the crystal planes (hkl) and is normal to these planes. The separation between these planes is 2π times the inverse of G .

(3) Now we are ready to show that the diffraction condition (2.13) is equivalent to the Bragg law (2.2). It follows from Eqs. (2.13) and (2.16) that

$$2(2\pi/\lambda)\sin\theta = 2\pi/d, \quad (2.17)$$

or $2d\sin\theta = \lambda$, where θ 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 the actual plane, because hkl may contain a common factor m , whereas in the definition of the Miller indices the common factor has been eliminated. Therefore, we can substitute $m\mathbf{G}$ instead of \mathbf{G} and obtain the Bragg result

$$2d\sin\theta = m\lambda. \quad (2.18)$$

Brillouin zones. Brillouin gave another statement of the diffraction condition.

Consider a two-dimensional lattice in the reciprocal space (Fig.5a). Let O be the origin of this lattice. Consider a reciprocal lattice vector, which connects points O and another reciprocal lattice site. Now draw the line (in the three dimensions it would be a plane), which is orthogonal to this vector and intercepts it in the midpoint. The x-ray will be diffracted if its wavevector \mathbf{k} has the magnitude and direction that is required by the condition (2.13), which can be rewritten in the following way

$$\mathbf{k} \cdot \left(\frac{1}{2}\mathbf{G}\right) = \left(\frac{1}{2}\mathbf{G}\right)^2, \quad (2.19)$$

It is easy to see that any \mathbf{k} vector connecting the origin and the plane will satisfy the diffraction condition.

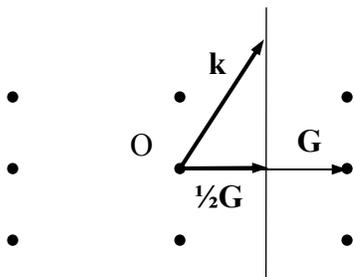


Fig.5a

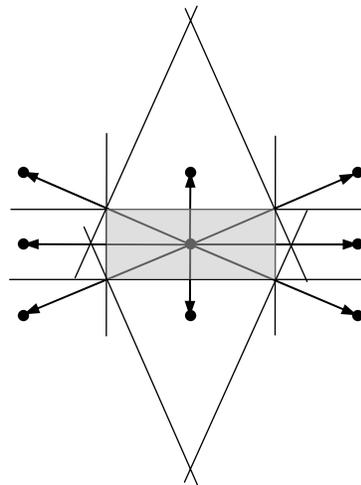


Fig.5b

In a similar way we can draw other lines (planes), which satisfy the diffraction condition. This is shown in Fig.5b. So the Brillouin construction exhibits all the wave vectors \mathbf{k} which can be Bragg-reflected by the crystal.

The central part of in the reciprocal lattice is of special importance in the theory of solids. It is the first Brillouin zone. The first Brillouin zone is the smallest volume entirely enclosed by the planes that are perpendicular bisectors of the reciprocal lattice vectors. In this construction it is the rectangle about the origin. The first Brillouin zone is the Wigner-Seitz primitive cell in the reciprocal lattice.

Two examples of the first Brillouin zone :

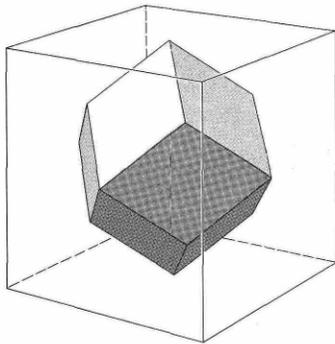
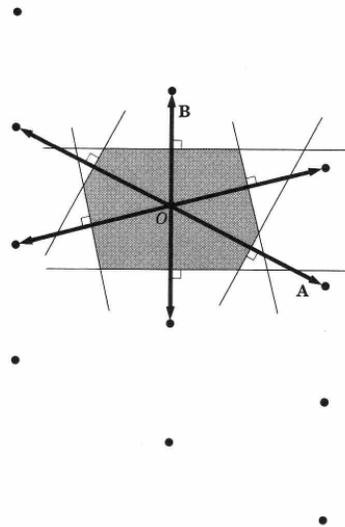


Fig.6

First Brillouin zone of the bcc lattice (rhombic dodecahedron).



First Brillouin zone of an oblique lattice in two dimensions.

Another alternative expression for the diffraction condition can be given in terms of *Lauer equations*. Taking a dot product of Eq.(2.5) with \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 we obtain:

$$\begin{aligned} \mathbf{a}_1 \cdot \Delta \mathbf{k} &= 2\pi m_1, \\ \mathbf{a}_2 \cdot \Delta \mathbf{k} &= 2\pi m_2, \\ \mathbf{a}_3 \cdot \Delta \mathbf{k} &= 2\pi m_3. \end{aligned} \tag{2.20}$$

These conditions state that the allowed scattering vectors, $\Delta \mathbf{k}$, should lie at intersections of cones around each lattice vector.

Diffraction amplitude. So far we have not discussed the amplitude and the width of diffraction peaks, which play an important role in the interpretation of x-ray diffraction data. This requires a more sophisticated analysis which we outline now.

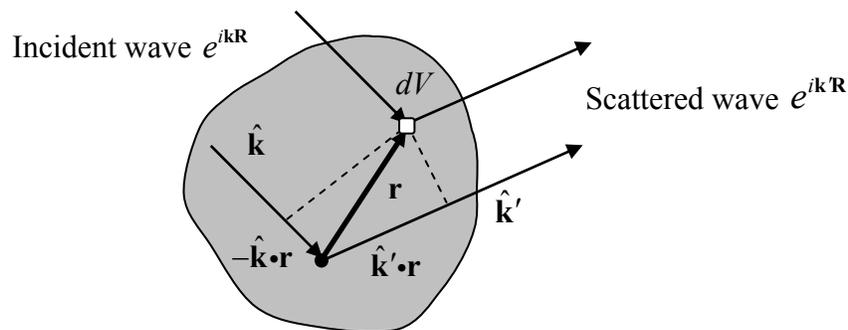


Fig.7

We consider scattering of x-rays by a solid as is shown in Fig.7. An incident plane wave $e^{i\mathbf{k}\cdot\mathbf{R}}$ (wave vector \mathbf{k}) is scattered, and a scattered wave $e^{i\mathbf{k}'\cdot\mathbf{R}}$ (wave vector \mathbf{k}') is detected. Scattering occurs due to the interaction of the incident x-rays with the electron charge distributed in a solid with charge density $n(\mathbf{r})$. The amplitude of scattering by an infinitesimal volume dV is proportional to the charge at this point, i.e. $n(\mathbf{r})dV$, and a phase factor $e^{i\Delta\phi}$ acquired by the scattered wave. The phase shift is equal to

$\Delta\phi = \mathbf{k}\cdot\mathbf{r} - \mathbf{k}'\cdot\mathbf{r} = -(\mathbf{k}' - \mathbf{k})\cdot\mathbf{r} = -\Delta\mathbf{k}\cdot\mathbf{r}$. The field at detector is the superposition of the waves scattered from all points of the sample, and, therefore, the total amplitude of scattering is given by

$$F = \int_{\text{solid}} dV n(\mathbf{r}) e^{-i\Delta\mathbf{k}\cdot\mathbf{r}}. \quad (2.21)$$

The intensity of detected radiation is proportional to $|F|^2$, and therefore F determines the intensity and the width of diffraction peaks.

In a perfect crystal the charge density $n(\mathbf{r})$ has translational periodicity same as the crystal lattice, i.e. it is invariant with respect to all the translations given by lattice vectors \mathbf{T} :

$$n(\mathbf{r}) = n(\mathbf{r} + \mathbf{T}). \quad (2.22)$$

This makes it possible to expand $n(\mathbf{r})$ in a Fourier series:

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}, \quad (2.23)$$

where the expansion is performed in reciprocal lattice vectors \mathbf{G} , and $n_{\mathbf{G}}$ is the Fourier component of the charge density given by the inverse Fourier transformation:

$$n_{\mathbf{G}} = \frac{1}{V} \int_V dV n(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}}, \quad (2.24)$$

here V is the volume of the solid.

Fourier series in one dimension. Recall that if function $f(x)$ is periodic so that $f(x) = f(x+a)$, where a is the period, then it can be expanded in Fourier series:

$$f(x) = f_0 + \sum_{p=1}^{\infty} C_p \cos\left(\frac{2\pi}{a} px\right) + \sum_{p=1}^{\infty} S_p \sin\left(\frac{2\pi}{a} px\right), \quad (2.25)$$

where p is an integer, and f_0 , C_p and S_p are the Fourier coefficients. This expansion can be rewritten in a more compact, exponential form:

$$f(x) = \sum_{p=-\infty}^{\infty} f_p \exp\left(i \frac{2\pi}{a} px\right), \quad (2.26)$$

in which the coefficients f_p are given in terms of f_0 , C_p and S_p . Defining $g = \frac{2\pi}{a} p$ we can write Eq.(2.26) as follows

$$f(x) = \sum_{g=-\infty}^{\infty} f_g \exp(igx), \quad (2.27)$$

where g 's can be considered as reciprocal lattice vectors of one dimensional lattice of period a . We see that Eq.(2.23) may be considered as generalization of Eq.(2.27) to three dimensions.

Now we show that expansion (2.23) is consistent with the condition of translational invariance (2.22):

$$n(\mathbf{r} + \mathbf{T}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot(\mathbf{r}+\mathbf{T})} = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} e^{i\mathbf{G}\cdot\mathbf{T}} = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} = n(\mathbf{r}), \quad (2.28)$$

where we took into account that $e^{i\mathbf{G}\cdot\mathbf{T}} = 1$ due to Eq.(2.6).

The amplitude of scattering (2.24) has maxima corresponding to the diffraction condition (2.5). Indeed, substituting Eq.(2.23) in Eq.(2.21) we obtain:

$$F = \sum_{\mathbf{G}} n_{\mathbf{G}} \int_V dV e^{i(\mathbf{G}-\Delta\mathbf{k})\cdot\mathbf{r}} . \quad (2.29)$$

If $\Delta\mathbf{k} = \mathbf{G}_0$, where \mathbf{G}_0 is a particular reciprocal lattice vector, the amplitude of scattering (2.29) is equal to $F = Vn_{\mathbf{G}_0}$, otherwise it is negligibly small. Therefore, the intensity of a Bragg peak is determined by a respective Fourier component of the charge density $n_{\mathbf{G}_0}$.

Scattering from a lattice with basis. If the crystal structure represents a lattice with a basis, then we should take into account scattering by the atoms which have non-equivalent positions in a unit cell. The intensity of radiation scattered in a given Bragg peak will depend of the extent to which the rays scattered from these basis sites interfere with one another. To take into account basis atoms, first, let us rewrite Eq. (2.21) for the scattering amplitude at the diffraction condition, $\Delta\mathbf{k} = \mathbf{G}$, in terms of the integral over a unit cell:

$$F = \sum_{\mathbf{T}} \int_{cell} dV n(\mathbf{r} + \mathbf{T}) e^{-i\mathbf{G}\cdot(\mathbf{r}+\mathbf{T})} , \quad (2.30)$$

where the sum is taken over all the lattice vectors \mathbf{T} . Taking into account that $n(\mathbf{r} + \mathbf{T}) = n(\mathbf{r})$ and that $e^{i\mathbf{G}\cdot\mathbf{T}} = 1$, we obtain

$$F = \sum_{\mathbf{T}} \int_{cell} dV n(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} = N \int_{cell} dV n(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} = NS_{\mathbf{G}} . \quad (2.31)$$

where N is the number of cells in the solid, and we defined the *structure factor*

$$S_{\mathbf{G}} = \int_{cell} dV n(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} . \quad (2.32)$$

Assuming that we have s atoms in a unit cell located at $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$, it is convenient to write charge density as the superposition of charge densities n_j associated with each atom j of the basis:

$$n(\mathbf{r}) = \sum_{j=1}^s n_j(\mathbf{r} - \mathbf{r}_j) . \quad (2.33)$$

The structure factor may now be written as

$$S_{\mathbf{G}} = \sum_{j=1}^s \int dV n_j(\mathbf{r} - \mathbf{r}_j) e^{-i\mathbf{G}\cdot\mathbf{r}} = \sum_{j=1}^s e^{-i\mathbf{G}\cdot\mathbf{r}_j} \int dV n_j(\boldsymbol{\rho}) e^{-i\mathbf{G}\cdot\boldsymbol{\rho}} . \quad (2.34)$$

where $\boldsymbol{\rho} \equiv \mathbf{r} - \mathbf{r}_j$. The integral in Eq.(2.34) is known as the *atomic form factor* :

$$f_j(\mathbf{G}) = \int dV n_j(\boldsymbol{\rho}) e^{-i\mathbf{G}\cdot\boldsymbol{\rho}} , \quad (2.35)$$

which is determined by the charge density of atom j in the basis. The structure factor is then

$$S_{\mathbf{G}} = \sum_{j=1}^s f_j(\mathbf{G}) e^{-i\mathbf{G}\cdot\mathbf{r}_j} . \quad (2.36)$$

Example: structure factor of bcc lattice. A conventional cell of the bcc lattice contains two identical atoms with coordinates: $\mathbf{r}_1 = 0$ and $\mathbf{r}_2 = (a/2)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$. Since the atoms are identical the atomic form factors are same, i.e. $f_1 = f_2 = f$. The reciprocal unit cell is cubic with a cell side of $2\pi/a$, and the reciprocal vector is given by

$$\mathbf{G} = \frac{2\pi}{a}(m_1\hat{\mathbf{x}} + m_2\hat{\mathbf{y}} + m_3\hat{\mathbf{z}}) . \quad (2.37)$$

The structure factor is, then,

$$\begin{aligned} S_{\mathbf{G}} / f &= \exp(-i\mathbf{G}\cdot\mathbf{r}_1) + \exp(-i\mathbf{G}\cdot\mathbf{r}_2) = 1 + \exp\left[-i\frac{2\pi}{a}(m_1\hat{\mathbf{x}} + m_2\hat{\mathbf{y}} + m_3\hat{\mathbf{z}})\cdot\frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})\right] = \\ &= 1 + \exp[-i\pi(m_1 + m_2 + m_3)] = 1 + (-1)^{m_1+m_2+m_3} \end{aligned} \quad (2.38)$$

Therefore $S_{\mathbf{G}}=2f$, if $m_1+m_2+m_3$ is even, and $S_{\mathbf{G}}=0$, if $m_1+m_2+m_3$ is odd.

Thus, diffraction peaks will be observed, e.g, from the (110), (200), (211) planes, but not from the (100), (111), (210) planes. The later fact is due to the destructive interference from the basis atoms which cancel some peaks. For example, as is seen from Fig.8 for the (100) plane, the phase difference between successive planes is π , so that the reflected amplitude from two adjacent planes is $1 + e^{-i\pi} = 0$.

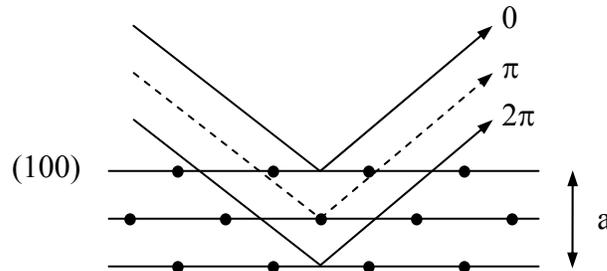


Fig.8

Structure factor of fcc lattice. The basis of the fcc structure referred to the cubic cell has identical atoms at $\mathbf{r}_1 = 000$; $\mathbf{r}_2 = \frac{1}{2}\frac{1}{2}0$; $\mathbf{r}_3 = 0\frac{1}{2}\frac{1}{2}$; $\mathbf{r}_4 = \frac{1}{2}0\frac{1}{2}$. Therefore,

$$S_{\mathbf{G}} / f = 1 + e^{-i\pi(m_2+m_3)} + e^{-i\pi(m_1+m_3)} + e^{-i\pi(m_1+m_2)} , \quad (2.39)$$

which is non-zero only if all the indices are even or all the indices are odd. Allowed peaks are, e.g., (111), (200), (222), (220), (131).

Atomic form factor. The atomic form factor is defined by Eq.(2.35). It depends on the number and distribution of atomic electrons, and on the wavelength and angle of scattering of the radiation. It measures the scattering power of j -th atom in the unit cell. An example of the importance of the atomic form factor is given below.

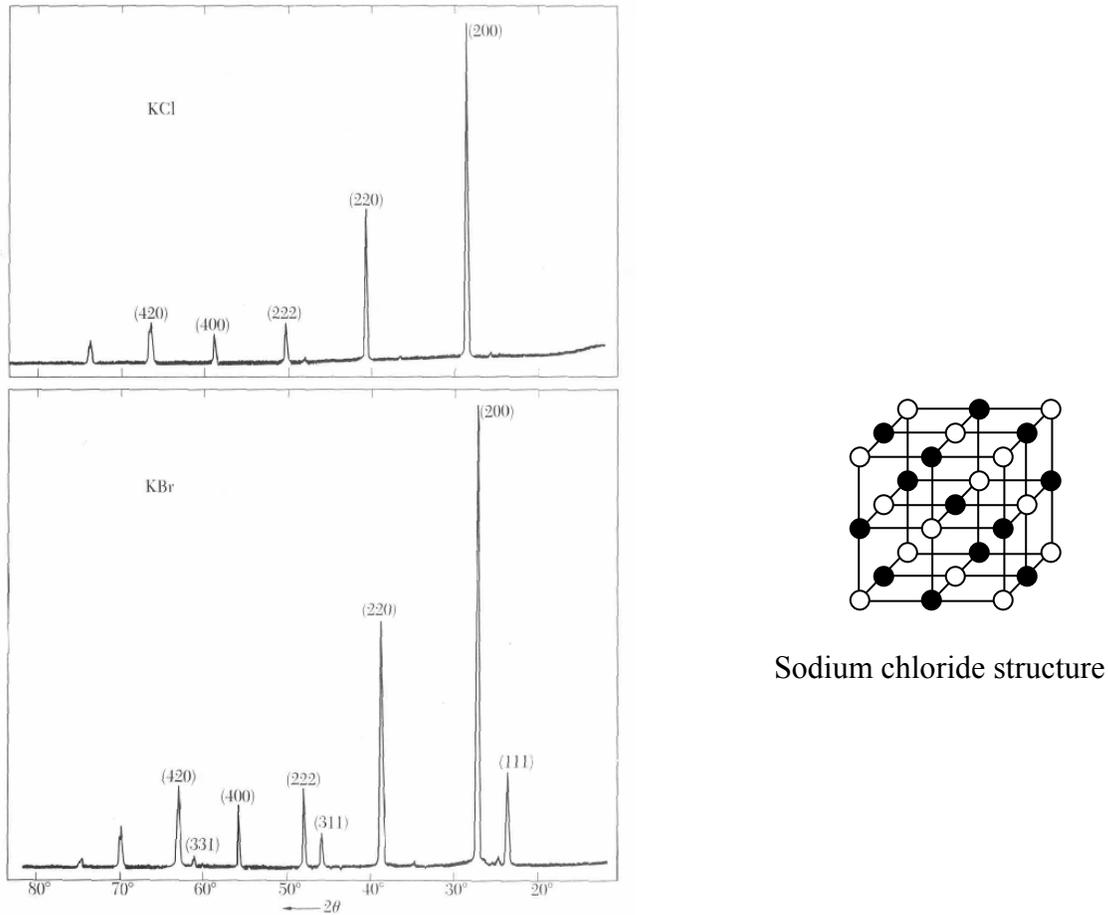


Fig. 8 (Figure 17 from Kittel). Comparison of x-ray reflections from KCl and KBr powders.

Both KCl and KBr have *sodium chloride structure* shown in the figure. In this structure the two types of atoms are arranged alternatively at the lattice sites of a simple cubic lattice. The space lattice is fcc with a basis of two non-equivalent atoms at 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

In KCl the number of electrons of K^+ and Cl^- ions are equal and the charge distribution is similar. Therefore, the form factors for K^+ and 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 than that of K^+ , and all reflections of the fcc lattice are present.