On the Problem of Observing the Maximum of a Superposition Wave Field

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Abstract. The well-known Laue condition determining the intensity maximums of diffracted on an ideal crystal structure plane wave is discussed. It is proved that the Laue conditions, which are restrictions imposed on the values of the scattering wave vector, is more correctly to be considered as a pair of two conditions. The first conditions relate to the wave vector of an incident wave and the second conditions relate to the wave vector of an observation direction. In other words, to observe the maximums, it is not enough that only the difference (the scattering wave vector) of these two vectors satisfies the Laue condition. To observe the maximums, it is necessary that each of these vectors separately, i.e. the wave vector of the incident wave and the wave vector of the observation direction, satisfy the Laue condition. It is shown that such a doubling of the maximums conditions leads to a decrease in the number of observed maximums compared to the condition imposed only on the scattering wave vector.

Keywords: far field diffraction, ideal structure, Laue conditions

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1. Introduction

Despite the long-standing solution the problem of describing a diffracted flat field on an ideal periodic structure in the far observation zone, the results of Laue [1] remain relevant to this day [2-15]. As it is known, the Laue conditions correspond to the kinematic picture of diffraction, when in the crystal volume the re-emitted field is considered to be significantly smaller than the primary field, which, as a rule, is considered in the form of a plane wave. According to Laue's conditions in the Fraunhofer approximation, the positions of the main maximums, when the intensity of the diffracted field takes on the maximum possible value, can be identified on the basis of certain restrictions imposed on the values and directions of the scattering wave vector:

$$\vec{q}\vec{a} = 2\pi l_a,\ \vec{q}\vec{b} = 2\pi l_b,\ \vec{q}\vec{c} = 2\pi l_c\ \ (l_a,\ l_b,\ \ l_c = 0, \pm 1, \pm 2, \cdots), \tag{1}$$

where $\vec{q}$ - the scattering wave vector and the quantities $\vec{a}, \vec{b}, \vec{c}$ are the translation vectors of the three-dimensional diffraction grating.

It is clear that the positions of the atoms in the crystal will be determined by the vectors

$$\vec{r}_{nmh} = \vec{a} \cdot n + \vec{b} \cdot m + \vec{c} \cdot h, \tag{2}$$

and if

$$n = 1, 2, \cdots, N_a,\ m = 1, 2, \cdots, N_b,\ h = 1, 2, \cdots, N_c\,, \tag{3}$$

then the volume of the crystal is represented by a parallelepiped, with sides $(N_a - 1)a$, $(N_b - 1)b$, $(N_c - 1)b$ and with the number of atoms

$$N = N_a N_b N_c . \tag{4}$$

The expression for the intensity of the diffracted field is also well known (see, for example, [16]):

$$I(N) = \frac{1}{2}\left(\frac{A}{R_0}\right)^2 \frac{\sin^2\left[\frac{\vec{q}\vec{a}}{2}N_a\right]}{\sin^2\left[\frac{\vec{q}\vec{a}}{2}\right]} \frac{\sin^2\left[\frac{\vec{q}\vec{b}}{2}N_b\right]}{\sin^2\left[\frac{\vec{q}\vec{b}}{2}\right]} \frac{\sin^2\left[\frac{\vec{q}\vec{c}}{2}N_c\right]}{\sin^2\left[\frac{\vec{q}\vec{c}}{2}\right]} . \tag{5}$$

Using (1) and (5) it is not difficult to see that the intensity at maximum takes the following value:

$$I_{\max} = \frac{1}{2}\left(\frac{A}{R_0}N_a N_b N_c\right)^2 = \frac{1}{2}\left(\frac{A}{R_0}N\right)^2 . \tag{6}$$

As it will be shown in this work, Laue’s conditions generally speaking do not reflect the entire necessary set of experimental conditions for observing the main maximums in diffraction experiments. As a more consistent consideration shows, condition (1) must be satisfied not only by the difference between the wave vectors of the incident wave and the observation direction (the scattering wave vector), but each of these vectors separately.

2. The intensity of a flat field diffracted on an ideal structure

Let a plane wave falls on an ideal crystalline structure with the positions of the atoms determined by translation vectors (see (2)):

$$\Phi(\vec{r}, t) = B\cos(\omega t - \vec{K}\vec{r}) , \tag{7}$$

where B is the amplitude of the primary plane wave, ω is the frequency, $\vec{K}$ is the wave vector of an illumination direction, $\vec{r}$ is a spatial vector. The diffracted field we will consider as a result of superposition of sphere waves generated by the crystal atoms under the action of the external field (7):

$$U(\vec{R}, t) = \sum_{n=1}^{N_a}\sum_{m=1}^{N_b}\sum_{h=1}^{N_c} \frac{A}{\left|\vec{R} - \vec{r}_{nmh}\right|} \cos\left[\omega t - k\left|\vec{R} - \vec{r}_{nmh}\right| + \gamma_{nmh}\right], \tag{8}$$

where γ_{nmh} - is the initial phase of a sphere wave generated by the atom located in the point mentioning by the vector $\vec{r}_{nmh}$. In the dipole approximation the quantities γ_{nmh} defined by means of the wave vector of the primary field (7) (see, for example, [16, 17]):

$$\gamma_{nmh} = -\vec{K}\,\vec{r}_{nmh}\,. \tag{9}$$

Let the screen of observation σ has a form of a flat plat which is perpendicular to the space vector $\vec{R}_0$ (see Fig. 1). We will call this vector as a mean observation vector and its module $R_0 = \left|\vec{R}_0\right|$ as the main observation distance. The end point of the $\vec{R}_0$ on the observation screen σ, i.e. the point O', we will call the center of the screen. Let the vector $\vec{\rho}$ starting from the screen center specifies the observation point. It is easy to see that between the vector $\vec{R}$ specifying the observation point from the coordinate system origin and the vector $\vec{\rho}$ specifying the observation point from the screen origin the following relation acts:

$$\vec{R} = \vec{R}_0 + \vec{\rho}\,. \tag{10}$$

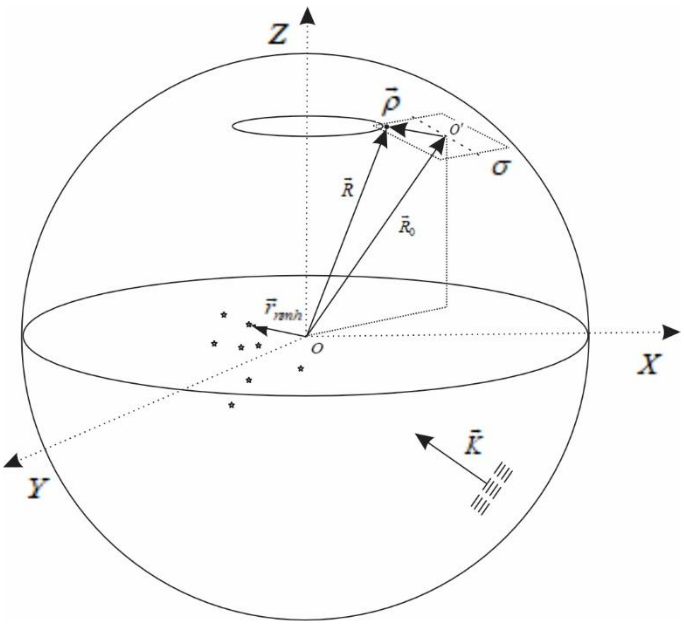

Fig. 1. To the problem of approximate description of a superposition filed of secondary sphere waves generated by a plane field.

Using the necessary conditions for the approximate description of the wave field (8):

$$\vec{r}^{\,2}_{nmh} << R_0^2\,,\ \vec{\rho}^{\,2} << R_0^2\,, \tag{11}$$

the amplitudes of the sphere waves can be considered equal to each other:

$$\frac{A}{\left|\vec{R}-\vec{r}_{nmh}\right|} = \frac{A}{\left|\vec{R}_0+\vec{\rho}-\vec{r}_{nmh}\right|} \approx \frac{A}{R_0}\,, \tag{12}$$

Taking into account (12) and (9) the intensity of the wave field (8) on the observation screen can be presented as:

$$I(N)=\frac{1}{2}\left(\frac{A}{R_0}\right)^2\sum_{n=1}^{N_a}\sum_{n'=1}^{N_a}\sum_{m=1}^{N_b}\sum_{m'=1}^{N_b}\sum_{h=1}^{N_c}\sum_{h'=1}^{N_c}\cos^2\left[\frac{k\left(\left|\vec{R}-\vec{r}_{nmh}\right|-\left|\vec{R}-\vec{r}_{n'm'h'}\right|\right)-\vec{K}\left(\vec{r}_{n'm''h}-\vec{r}_{nmh}\right)}{2}\right]. \quad (13)$$

For many problems of the wave theory the investigation of the sum (13) is more productively to conduct in the so called Fraunhofer pattern, when

$$\frac{\left|\vec{r}_{nmh}\right|^2}{\lambda R_0}<<1,\ \frac{\left|\vec{\rho}\right|^2}{\lambda R_0}<<1, \quad (14)$$

where $\lambda=2\pi/k$ is the wave length. Note that (11) is necessary condition and (14) is sufficient condition for applying the Fraunhofer approximation. In the case of fulfillment of (11), (14) the intensity (13) takes the form of (see, for example, [18]):

$$I(N)=\frac{1}{2}\left(\frac{A}{R_0}\right)^2\sum_{n=1}^{N_a}\sum_{n'=1}^{N_a}\sum_{m=1}^{N_b}\sum_{m'=1}^{N_b}\sum_{h=1}^{N_c}\sum_{h'=1}^{N_c}\cos^2\left[\frac{\vec{q}(\vec{r}_{nmh}-\vec{r}_{n'm'h'})}{2}\right], \quad (15)$$

where

$$\vec{q}=\vec{K}-\vec{k} \quad (16)$$

is the scattering wave vector and the quantity $\vec{k}$ is the wave vector corresponding to the main observation direction:

$$\vec{k}=k\vec{R}_0/R_0 \text{ and } \left|\vec{k}\right|=\left|\vec{K}\right|=k. \quad (17)$$

One can check that in the case of (2) the value of the sum (15) is given by the expression (5). From (15) it directly follows that when

$$\vec{q}(\vec{r}_{nmh}-\vec{r}_{n'm'h'})=2\pi l\ \ (l=0,\pm1,\pm2,\cdots), \quad (18)$$

then the intensity takes the maximum value (see (6)). Since the quantity $\vec{a},\vec{b},\vec{c}$ are independent from each other one can see that the condition (18) is equivalent the Laue conditions (1):

$$l=l_a+l_b+l_c. \quad (19)$$

Here it is necessary to pay special attention to one important circumstance, which obviously falls out in an approximate consideration of the superposition field (13). The fact is that if one was guided by the expression of the field in the form of sum (13), where the expressions for the phases of spherical waves are exact, then it is easy to see that the maximum condition decomposes into two conditions. Using (13) one can see that the intensity takes the maximum (6) if

$$\vec{K}\left(\vec{r}_{n'm''h}-\vec{r}_{nmh}\right)-k\left(\left|\vec{R}-\vec{r}_{nmh}\right|-\left|\vec{R}-\vec{r}_{n'm'h'}\right|\right)=2\pi l\ \ (l=0,\pm1,\pm2,\cdots). \quad (20)$$

The given condition can be satisfied if only the following two conditions take place:

$$\vec{K}\left(\vec{r}_{n'm''h}-\vec{r}_{nmh}\right)=2\pi H \;\; (H=\pm1,\pm2,\cdots), \tag{21}$$

$$k\left(\left|\vec{R}-\vec{r}_{nmh}\right|-\left|\vec{R}-\vec{r}_{n'm'h'}\right|\right)=2\pi h \;\; (h=\pm1,\pm2,\cdots), \tag{22}$$

so that

$$l=H+h.$$

The conditions (21) we will call the illumination condition and the condition (22) as the observation condition. Note that for a maximum observation the both condition should be fulfillment.

In is important to mention that in contrast to the number l (see (20)) the numbers H,h do not take the zero value, since $k\neq 0$ (see (17) as well). One can check that in the case of the Fraunhofer approximation (see (11), (14)) the equality (22) takes the form of (see, for example, [17]):

$$\vec{k}\left(\vec{r}_{n'm''h}-\vec{r}_{nmh}\right)=2\pi h. \tag{23}$$

One can see that in the case of the Fraunhofer approximation the wave vector of the observation direction $\vec{k}$ satisfies to the condition similar to the condition written for the wave vector of the primary plane wave $\vec{K}$ (21). It is important to note that the condition for the vector $\vec{K}$ does not depend on an approximation [18].

As follows from the above, even in the Fraunhofer case, for observation of a maximum two conditions must be satisfied: first of them for the vector $\vec{K}$ (see (21)) and second one for the vector $\vec{k}$ (23). It is obvious that the condition (18) follows from the conditions (21), (23) ($l=H+h$), while the converse is not true.

3. The generalized Laue conditions

As it was shown above the Laue condition written for the scattering wave vector $\vec{q}$ (see (1) or (18)) is not a complete condition for observing the maximum. To observe the maximum, it is necessary that both vectors $\vec{K}$, $\vec{k}$ separately correspond to the multiplicity condition of the difference of phases to 2π. Let us consider the following vectors:

$$\vec{K}^{\max}=M\cdot\vec{a}^{*}+P\cdot\vec{b}^{*}+S\cdot\vec{c}^{*}\,(M,P,S=0,\pm1,\pm2,\cdots), \tag{24}$$

$$\vec{k}^{\max}=m\cdot\vec{a}^{*}+p\cdot\vec{b}^{*}+s\cdot\vec{c}^{*}\;(m,p,s=0,\pm1,\pm2,\cdots), \tag{25}$$

where

$$\vec{a}^{*}=2\pi\frac{\left[\vec{b}\times\vec{c}\right]}{\vec{a}\cdot\left[\vec{b}\times\vec{c}\right]},\;\vec{b}^{*}=\frac{\left[\vec{c}\times\vec{a}\right]}{\vec{b}\cdot\left[\vec{c}\times\vec{a}\right]},\;\vec{c}^{*}=2\pi\frac{\left[\vec{a}\times\vec{b}\right]}{\vec{c}\cdot\left[\vec{a}\times\vec{b}\right]}. \tag{26}$$

One can see that the vectors $\vec{K}^{\max}$ and $\vec{k}^{\max}$ satisfy to the conditions (21) and (23) correspondingly. Therefore these vectors are mentioned by the upper index *max*. Note that in constant to the number

H (see (21)) the numbers M,P,S (see (24)) can also be equal to zero, but not simultaneously. The same can be said about the numbers h and m,p,s appearing in the formulas (23) and (25).

The vectors (26) are nothing more than the well-known translation vectors of an inverse lattice. Note that all three denominators in fractions (26) are equal to each other:

$$\vec{a}\cdot\left[\vec{b}\times\vec{c}\right]=\vec{b}\cdot\left[\vec{c}\times\vec{a}\right]=\vec{c}\cdot\left[\vec{a}\times\vec{b}\right]=V\,, \tag{27}$$

and are equal to the volume of the parallelepiped built on the basis of the vectors $\vec{a},\vec{b},\vec{c}$. It is interesting to consider the inverse to (26) formulas expressing the basis vectors of the direct lattice by mean of the basic vectors $\vec{a}^*$, $\vec{b}^*$, $\vec{c}^*$ of the inverse lattice:

$$\vec{a}=2\pi\frac{\left[\vec{b}^*\times\vec{c}^*\right]}{\vec{a}^*\cdot\left[\vec{b}^*\times\vec{c}^*\right]},\ \vec{b}=2\pi\frac{\left[\vec{c}^*\times\vec{a}^*\right]}{\vec{b}^*\cdot\left[\vec{c}^*\times\vec{a}^*\right]},\ \vec{c}=2\pi\frac{\left[\vec{a}^*\times\vec{b}^*\right]}{\vec{c}^*\cdot\left[\vec{a}^*\times\vec{b}^*\right]}. \tag{28}$$

It is obvious that the knowledge of the vectors $\vec{a}^*$, $\vec{b}^*$, $\vec{c}^*$ allows to define the elementary translation vectors of a direct lattice. In its turn when the pattern of the maximums is appeared the vectors $\vec{a}^*$, $\vec{b}^*$, $\vec{c}^*$ linearly connection with the wave vectors of illumination $\vec{K}^{\max}$ and observation $\vec{k}^{\max}$ (see (24), (25)). The above means that the translation vectors $\vec{a},\vec{b},\vec{c}$ can be determined by means of the vectors $\vec{K}^{\max}$, $\vec{k}^{\max}$. So the problem is reduced to determination of vectors $\vec{a}^*$, $\vec{b}^*$, $\vec{c}^*$ by means of diffraction wave vectors $\vec{K}^{\max}$ and $\vec{k}^{\max}$.

Further, for convenience, we will omit the index *max* of the wave vectors of the maximums (see (24), (25)) and will mark them with the corresponding indices:

$$\vec{K}^{\max}\equiv\vec{K}_{MPS}\ ,\ \vec{k}^{\max}=\vec{k}_{mps}\,. \tag{29}$$

Taking into account (29) and (24), (25) one can get

$$\vec{K}_{MPS}\vec{a}=2\pi M\,,\ \vec{K}_{MPS}\vec{b}=2\pi P\,,\vec{K}_{MPS}\vec{c}=2\pi S\,, \tag{30}$$

$$\vec{k}_{mps}\vec{a}=2\pi m\,,\ \vec{k}_{mps}\vec{b}=2\pi p\ ,\ \vec{k}_{mps}\vec{c}=2\pi s\,. \tag{31}$$

Due to the fact that (see (17))

$$\left|\vec{K}_{MPS}\right|=\left|\vec{k}_{mps}\right|=k=2\pi/\lambda\ , \tag{32}$$

the inverse lattice node indicated by the vectors $\vec{K}_{MPS}$, $\vec{k}_{mps}$ must be located on a sphere of radius $2\pi/\lambda$:

$$\left(M\cdot\vec{a}^*+P\cdot\vec{b}^*+S\cdot\vec{c}^*\right)^2=\left(m\cdot\vec{a}^*+p\cdot\vec{b}^*+s\cdot\vec{c}^*\right)^2=4\pi^2/\lambda^2\,. \tag{33}$$

Note that in the diffraction theory of X-rays the sphere of radius of $2\cdot(2\pi/\lambda)$ is known as the Ewald's sphere:

$$\left|\vec{q}_{MPS}^{mps}\right| = 4\pi/\lambda \ , \tag{34}$$

where $\vec{q}_{MPS}^{mps}$ is corresponding scattering wave vector, when the illumination is done upon the direction of the inverse lattice vector $\vec{K}_{MPS}$ and the intensity observation is conducted over the inverse lattice vector $\vec{k}_{mps}$:

$$\vec{q}^{\max} \equiv \vec{q}_{MPS}^{mps} = \vec{K}_{MPS} - \vec{k}_{mps} . \tag{35}$$

Taking into (35) and (24), (25) one can check that

$$\vec{q}^{\max} = l_a\vec{a}^* + l_b\vec{b}^* + l_c\vec{c}^* , \tag{36}$$

where

$$l_a = M - m,\ l_b = P - p,\ l_c = S - s . \tag{37}$$

Taking into account (35)-(37) from (30), (31) one can get the well-known Laue conditions for determination of diffraction maximums:

$$\vec{q}^{\max}\vec{a} = 2\pi l_a,\ \vec{q}^{\max}\vec{b} = 2\pi l_b\ ,\ \vec{q}^{\max}\vec{c} = 2\pi l_c . \tag{38}$$

As consideration made above the given conditions do not reflect the entire set of conditions required to observe maximums. The equalities (38) can be considered as a necessary condition for the diffraction maximums. In accordance with conditions (30), to observe the maximums, the crystal illumination must also be carried out in an appropriate manner, i.e. the wave vector $\vec{K}_{MPS}$ of the elimination direction should be the inverse lattice vector as well.

4. Conclusions

Thus, we have proved that to observe the maximums, it is necessary that each of these vectors separately, i.e. the wave vector of the incident wave and the wave vector of the observation direction, satisfy the Laue condition. It is shown that such a doubling of the maximums conditions leads to a decrease in the number of observed maximums compared to the condition imposed only on the scattering wave vector.

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