18 Conditions for directions of principal maxima at the diffraction by lattices. The Laue equations and the Bragg equation

It was explained in Section 2.1 that the wave function of the radiation diffracted by an object \( f(\vec{x}) \) in the direction \( \vec{n} = \vec{n}_0 + \vec{X} \) is specified by the Fourier transform \( F(\vec{X}) \) of the object \( f \) at the point the position vector of which is equal to scattering vetor \( \vec{X} \). Several of the previous chapters dealt with the Fourier transform of lattices. Thus, everything is prepared for the discussion of the diffraction by lattices. We shall start with the diffraction by a three-dimensional lattice.

We have seen that the Fourier transform of a lattice is the reciprocal lattice with the reciprocal constant \( K = \frac{2\pi}{k} \) (cf. Section 4.3). If the original lattice is finite, the lattice points of the reciprocal lattice are occupied by the shape amplitudes \( G_1(\vec{X}) \) (cf. 17(12)), which superpose to form the lattice amplitude \( G(\vec{X}) \) (cf. 17(13)). This lattice amplitude \( G(\vec{X}) \) is a periodic function and its absolute value takes its maximum just at the points \( \vec{X} = \frac{2\pi}{k} \vec{X}_h \) (cf. 17(5)). This is the fact of high priority, because the most important equations of structure analysis — the Laue equations and the Bragg equation — are its consequences. Namely, it says, that principal diffraction maxima have directions \( \vec{n}_h \), for which the scattering vector \( \vec{X} \) (cf. 2(1)) takes the values

\[
\vec{X} = \vec{n}_h - \vec{n}_0 = \frac{2\pi}{k} \vec{X}_h = \frac{2\pi}{k} (h_1 \vec{a}_1 + h_2 \vec{a}_2 + h_3 \vec{a}_3).
\]

Of course, here \( k \) is the wave number \( k = \frac{2\pi}{\lambda} \) and not a constant that can be chosen so freely as in the case of the Fourier transform. The reason is that \( k \) has the above meaning in the integral 2.1(8). The conditions for the directions \( \vec{n}_h \) of principal diffraction maxima are then given by

\[
\frac{\vec{n}_h - \vec{n}_0}{\lambda} = \vec{X}_h
\]

as known from reference books (see e.g. [1] p. 115).

![Figure 1: The Ewald construction. Crosses represent the shape amplitudes \( G_1 \) situated at lattice points of the reciprocal lattice.](image)

The geometrical interpretation of this condition is the Ewald construction, which is understood in the following way (cf. Figure 1):
(i) Using relations 4.2(7) we construct the reciprocal lattice to the lattice at which the diffraction takes place and situate the shape amplitudes $G_1$ at the reciprocal lattice positions. (When calculating $G_1$ from 17(7) and 17(8) we must use $k = 2\pi$ in 17(7)).

(ii) We construct spherical surface $\rho$ that passes through the origin $O$, has the radius $\frac{1}{\lambda}$, and its centre $C$ is determined by the condition $CO = \frac{\vec{n}_0}{\lambda}$ (the Ewald spherical surface).

(iii) From equation (2) then it follows that the diffraction maxima are in the directions $\vec{n}_h$ from the centre $C$ to those points $Q$ on the spherical surface $\rho$ that coincide with the reciprocal lattice points $\vec{X}_\vec{h}$.

Thus, the shapes of the diffraction spots represent the cross-sections through the squared modulus of the shape amplitudes $G_1$ situated at the reciprocal lattice points by the Ewald spherical surface $\rho$.

In this way the shapes of the diffraction spots inform us about the shape of the crystal from which the diffraction takes its rise. This may be utilized for the investigation of the shape of nanocrystals and of the initial stage of the crystallization [4]. Therefore the shape amplitudes of several basic polyhedra have been calculated (Appendix D, [5], [6], [7]).

The Laue equations [2] are another form of presentation of the condition (2). They can be derived by successive scalar multiplication of equation (2) by basis vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ of the lattice. With the use of 4.2(1) we get

\[
\begin{align*}
(\vec{n}_\vec{h} - \vec{n}_0) \cdot \vec{a}_1 &= h_1 \lambda, \\
(\vec{n}_\vec{h} - \vec{n}_0) \cdot \vec{a}_2 &= h_2 \lambda, \quad \text{i.e.} \\
(\vec{n}_\vec{h} - \vec{n}_0) \cdot \vec{a}_3 &= h_3 \lambda, \\
\cos \alpha_1 - \cos \alpha_0_1 &= \frac{h_1 \lambda}{\eta_1}, \\
\cos \alpha_2 - \cos \alpha_0_2 &= \frac{h_2 \lambda}{\eta_2}, \\
\cos \alpha_3 - \cos \alpha_0_3 &= \frac{h_3 \lambda}{\eta_3},
\end{align*}
\]

where $\alpha_{0_1}$ is the angle $(\vec{n}_0, \vec{a}_1)$, i.e. the angle between the direction of the incident radiation and the direction of the basis vector $\vec{a}_1$ of the lattice. Similarly, $\alpha_r$ is the angle $(\vec{n}_\vec{h}, \vec{a}_r)$, i.e. the angle between the direction of the diffraction maximum and the vector $\vec{a}_r$.

By comparison of the sizes of vectors in the two sides of equation (2) the well-know Bragg equation [3] is obtained: It is evident from the Figure 2 that $|\vec{n}_\vec{h} - \vec{n}_0| = 2\sin \vartheta$ and it is known from the lattice geometry (see e.g. Appendix C, eq. (5)) that

\[
X_\vec{h} = \frac{1}{d_\vec{h}^2},
\]

where $d_\vec{h}$ is the spacing of lattice planes with Miller indices $(h_1,h_2,h_3)$. Hence, it follows from (2)

\[
\lambda = 2d_{h_1h_2h_3} \sin \vartheta.
\]

It is evident from the Ewald construction (Figure 1) that the Ewald spherical surface need not pass through any other reciprocal lattice point except the origin $O$. Consequently, it may happen that even if $\lambda < 2\alpha_r$ there are no principal diffraction maxima. The same is evident from the Laue equations (3) because they represent three equations for three direction cosines of the direction of the principal diffraction maximum. There is, however, further condition: the direction cosines are coordinate of the unit vector $\vec{n}_\vec{h}$. Thus, we have four conditions for three quantities $\cos \alpha_r$ which, generally, cannot be satisfied for certain $\lambda$ and integers $h_1, h_2, h_3$. 

Figure 2: To the derivation of the Bragg equation.
In the X–ray diffraction various subterfuges are used to get principal diffraction maxima ([8], [9]). At the Laue method the radiation with continuous wavelength spectrum is incident onto the single crystal specimen and condition (2) is satisfied by radiation of certain wavelength. The individual diffraction spots are originated by X–rays of different wavelengths. If monochromatic radiation is employed for the study of single crystal specimen it is necessary to move with the specimen to change continuously the orientation of the single crystal with respect to the incident beam (rotation method, the Weisenberg method, precession method). With the rotating crystal it rotates also the reciprocal lattice and condition (2) is always satisfied for an orientation of the reciprocal lattice vector $\vec{X}_h$. When studying a polycrystalline or powder specimen the situation is similar. The incident radiation is monochromatic and there are always so oriented single crystal grains in the specimen that condition (2) is satisfied and the diffraction pattern (Debyegram) arrises.

In HEED (high energy electron diffraction) the electrons have the wavelength by two orders shorter than the lattice parameters. The radius of the Ewald spherical surface $\rho$ is then so large compared with the reciprocal lattice parameters that the spherical surface $\rho$ may be replaced at the origin $O$ by the tangential plane $\tau$ (cf. Figure 3). Moreover, the specimens are thin and, therefore, the shape amplitudes have the form of needles perpendicular to the specimen. Consequently, considerable intensity is observed in directions $\overline{CQ}$ even if the vector $O\overline{Q}$ differs from the reciprocal lattice vector $\vec{X}_h = O\overline{Q}'$ (see Figure 3). The diffraction pattern may then be considered — at least in its central region — to be a plane cross–section through the reciprocal lattice (the deviation $Q'Q''$ is small compared to the reciprocal lattice parameters).

Figure 3: Approximation of the Ewald spherical surface $\rho$ by the tangential plane $\tau$ at HEED ($\lambda \ll a_r$).
References


