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On the Theory of the Bragg Reflection in the Case of Multiple X-Ray Diffraction

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A general theory of multiple X-ray diffraction in the Bragg geometry is formulated. Special attention is paid to obtain simple and compact formulae which are convenient for computer programming. Two cases are considered: the incident beam is either a plane-wave or a spherical-wave, and the reflection occurs either at one surface or at several surfaces of the same crystal. The theory allows to calculate the angular and spectral characteristics of the many-beam X-ray monochromators and interferometers in a general case. Results of the numerical calculation of the reflection coefficients are described for the three-beam (111/11$\bar{1}$) case of the CuK_α-radiation diffraction in silicon.

Es wird eine allgemeine Theorie der Mehrfach-Röntgenbeugung in Bragg-Geometrie formuliert. Insbesondere wird eine einfache und geschlossene Formel erhalten, die eine bequeme Computerprogrammierung gestattet. Zwei Fälle werden betrachtet: der einfallende Strahl ist entweder eine ebene Welle oder eine Kugelwelle, und die Reflexion tritt entweder an einer Oberfläche oder an einigen Oberflächen desselben Kristalls auf. Die Theorie erlaubt, die Winkel- und Spektralcharakteristiken der Mehrstrahl-Röntgenmonochromatoren und Interferometer im allgemeinen Fall zu berechnen. Die Ergebnisse der numerischen Berechnung der Reflexionskoeffizienten werden für den Dreistrahl (111/11$\bar{1}$)-Fall der CuK_α-Strahlenbeugung in Silizium beschrieben.

1. Introduction

Since 1965 when Borrmann and Hartwig observed the enhancement of the anomalous transmission in the many-beam region of angles, the interest in the multiple X-ray diffraction has continuously increased. However, many papers which have been published during these years, both experimental and theoretical, have been devoted mainly to the case of the X-ray diffraction in the Laue geometry when all radiation passes through the crystal. Among the few investigations on the many-beam Bragg reflection we want to mention the papers on the Renninger effect and the possibility connected with it to measure precisely the lattice parameter of a crystal [1, 2]. But in these works the knowledge of the exact character of the angular dependence of the many-beam reflection does not play an essential role. Therefore, the theoretical study of this phenomenon was not stimulated by these works.

Quite another situation arose in recent time when papers were published in which devices, using the many-beam Bragg reflection for obtaining a closed trajectory of X-rays were suggested. One can mention, for example, the three-beam X-ray interferometer by Graeff and Bonse [3] and also the X-ray resonator [4]. It is essential that in the many-beam region of angles energy can be transferred from any beam to any other one of the many-beam set by choosing the corresponding reflection surface. On the one hand one can solve the problem of beam splitting and following recombination and on the other hand, reduce the angular divergency and carry out the mono-

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chromatization of the incident beam by choosing the proper transition with the use of the reflection at various surfaces of the same crystal.

For finding the optimum variants solving these problems the theoretical investigation of the phenomenon of the many-beam Bragg reflection becomes very important. The present paper is devoted just to this question. As it is known, the consecutive calculation and analysis of both the dispersion surface and the reflection coefficients in the many-beam region of angles can be carried out only by numerical methods. Therefore, such a formulation of the dynamical theory of many-beam scattering is necessary that is convenient for a computer program to be worked out. For the Laue case this question has been analysed in [5] in which the scattering matrix has been determined and the problem has been reduced to the eigenvalue problem of this matrix.

In Section 2 the results of [5] are generalized for the Bragg-reflection case. The results of the numerical calculation of both reflection and transmission coefficients for the three-beam (111/11$\bar{1}$) case are described in Section 3. In Section 4 a general formula is obtained which describes the case of reflection at several surfaces of the same crystal. This formula is a basic one for the calculation of many-beam monochromators. The incident-spherical-wave approach was shown [6, 7] to be a basis for the calculation of the diffraction pattern when investigating the coherent phenomena which arise in X-ray diffraction with fixing the diffraction pattern on a film. The spherical-wave theory of the Bragg reflection is developed in Section 5.

2. Reflection of a Plane Wave at One Crystal Surface

Let a monochromatic plane wave with the wave vector $\boldsymbol{k}_0$ and the frequency ω fall on a crystal plate of thickness t. Let $\boldsymbol{n}$ be the normal to the plate surface directed towards the plate. It is necessary for observing multiple diffraction that the vector $\boldsymbol{k}_0$ is approximately equal to the vector $\boldsymbol{\varkappa}_0$ with the length $\varkappa_0 = \omega_0/c$ (c is the light velocity) and direction satisfying the Bragg condition for any set of reciprocal lattice vectors $\boldsymbol{h}_m$ simultaneously, namely

$$\boldsymbol{\varkappa}_m = \boldsymbol{\varkappa}_0 + \boldsymbol{h}_m\,, \qquad \varkappa_m^2 = \varkappa_0^2\,. \tag{2.1}$$

We assume that the incident radiation is slightly nonmonochromatic and has some angular divergence. Then ω_0 is the frequency corresponding to the intensity maximum of the radiation spectrum and the vector $\boldsymbol{k}_0$ can be expressed in the form

$$\boldsymbol{k}_0 = \boldsymbol{\varkappa}_0 + \boldsymbol{q}_0\,, \qquad \boldsymbol{q}_0 = \varkappa_0(\theta_1\boldsymbol{e}_1 + \theta_2\boldsymbol{e}_2 + \theta_\omega\boldsymbol{s}_0)\,. \tag{2.2}$$

Here $\boldsymbol{s}_0$ is the unit vector directed along $\boldsymbol{\varkappa}_0$, $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are the mutually perpendicular unit vectors lying in the plane perpendicular to $\boldsymbol{s}_0$. The parameters θ_1 and θ_2 characterize the angular deviation of the wave vector of the incident beam from the Bragg direction $\boldsymbol{s}_0$, and $\theta_\omega = (\omega - \omega_0)/\omega_0$ characterizes the relative frequency shift.

To describe the electromagnetic field of X-rays inside a crystal, we use Maxwell's equations for Fourier components of an electrical field vector $\boldsymbol{E}(\boldsymbol{k}, \omega)$. As usual, expressing the current density induced by the electromagnetic wave through the electric field vector and preserving only strong waves, we obtain a set of linear homogeneous equations for scalar amplitudes of the strong wave (for more detail see [5]). The complete X-ray radiation field can be written in the form

$$\boldsymbol{E}_s(r) = \mathrm{e}^{i\boldsymbol{k}_0\boldsymbol{r}}\, A_s(\omega) \sum_j \lambda_s(j, t)\, \mathrm{e}^{i\varepsilon_j z/2} \sum_{ms'} \sqrt{\frac{\gamma_0}{\gamma_m}}\, \mathrm{e}^{i\boldsymbol{h}_m(\boldsymbol{r}-\boldsymbol{r}_1)}\, B_{ms'}(j)\, \boldsymbol{e}_{ms'}\,. \tag{2.3}$$

Here $z = (\boldsymbol{r} - \boldsymbol{r}_1)\,\boldsymbol{n}$, $\boldsymbol{r}_1$ is the coordinate of a point lying on the entrance surface of the crystal, $\gamma_m = \boldsymbol{s}_m\boldsymbol{n}$, $\boldsymbol{s}_m$ is a unit vector along $\boldsymbol{\varkappa}_m$. The quantities $B_{ms}(j)$ and ε_j are the eigenvectors and eigenvalues of the scattering matrix $G_{mn}^{ss'}$,

$$\sum_{ns'} G_{mn}^{ss'} B_{ns'}(j) = \varepsilon_j B_{ms}(j) \,. \tag{2.4}$$

$A_s(\omega)$ is the amplitude of the incident plane-polarized wave in the polarization state s ($s = \pi, \sigma$), $\boldsymbol{e}_{ms}$ are the unit vectors lying in the plane perpendicular to $\boldsymbol{s}_m$ and determining the polarization state for the wave m.

The polarization vectors $\boldsymbol{e}_{ms}$ can be chosen in an arbitrary way. We are interested in the systematic multiple diffraction [8] when all the reciprocal lattice vectors lie in the same plane. In this case the vectors $\boldsymbol{e}_{ms}$ suggested in [9] are most convenient, namely, all the vectors $\boldsymbol{e}_{m\sigma}$ lie in the same plane as the vectors $\boldsymbol{h}_m$ and $\boldsymbol{e}_{m\pi}$ are determined from the condition that the vectors $\boldsymbol{e}_{m\pi}$, $\boldsymbol{e}_{m\sigma}$, and $\boldsymbol{s}_m$ form a right-handed system of orthogonal directions.

The scattering matrix G is determined through the Fourier components of a complex polarizability tensor χ.The expression for χ with account of all possible interactions between the X-rays and the crystal, has been obtained in [10]. Taking into consideration only the main contributions to χ, namely, Thomson scattering and the dipole part of a photoelectric absorption, we have [5, 7], according to (2.3)

$$G_{mn}^{ss'} = \frac{1}{\sqrt{\gamma_m \gamma_n}} \varkappa_0 \chi_{m-n} (\boldsymbol{e}_{ms} \boldsymbol{e}_{ns'}) - \alpha_m \delta_{mn}^{ss'} \,, \tag{2.5}$$

where

$$\alpha_m = \frac{2\boldsymbol{h}_m \boldsymbol{q}_0}{\varkappa_0 \gamma_m} \tag{2.6}$$

is a parameter characterizing the deviation from the Bragg condition for the beam m.

In the present work, we consider the cases in which at least one of the quantities γ_m is negative, i.e. the plane-wave with the wave vector $\boldsymbol{k}_m$ goes out of the crystal through the entrance surface (reflection). It is natural to refer all these cases to the Bragg reflection even if several of the diffracting waves pass through the crystal. Indeed, due to the presence of a multiplier $(\gamma_m \gamma_n)^{-1/2}$ the matrix G_r describing the scattering in a nonabsorbing crystal becomes nonhermitian. Therefore, it can have a complex eigenvalue for which the field diminishes exponentially when it penetrates into the crystal. This phenomenon is known in the two-wave case and arises just in the case of Bragg reflection.

The quantities $\lambda_s(j, t)$ determine the value of an excitation of the j-th mode of Bloch waves. They are defined by boundary conditions on both entrance and exit crystal surfaces. After averaging over a region with linear dimensions much greater than an interatomic distance a, we obtain, as usual, the boundary conditions for each m-th beam in the superposition (2.3) separately. Then the amplitude of the Bragg-reflected beams has to vanish on the exit surface of the crystal plate $z = t$ and the amplitude of Laue diffracted beams has to be equal to zero on the entrance surface $z = 0$. These conditions are conveniently written in the form

$$\sum_j c_m(j, t)\, B_{ms'}(j)\, \lambda_s(j, t) = \delta_{m0} \delta_{ss'} \,, \tag{2.7}$$

where

$$c_m(j, t) = \begin{cases} 1; & \gamma_m > 0 \,, \\ \exp\,[i\varepsilon_j t/2]; & \gamma_m < 0 \,. \end{cases} \tag{2.8}$$

The set (2.4) does not define the length of the vectors B_{ms}, but the general field (2.3) according to (2.7) does not depend on the choice of the length of the vectors. The vectors are conveniently normalized to unity. The eigenvalue problem (2.4) in the many-beam case with any value of the vector $\boldsymbol{q}_0$ can be solved only by numerical methods using a computer. We note that, contrary to the Laue case, the methods of diagonalization of nonhermitian matrices have to be used here.

If the crystal has an inversion centre in the point $\boldsymbol{Q}_0$ then it is easy to verify directly that the substitution $B_{ms} = \tilde{B}_{ms} \exp(-i\boldsymbol{h}_m\boldsymbol{Q}_0)$ gives the symmetrical complex matrix $\tilde{G}$. For the numerical diagonalization of this matrix the method of complex rotations was found to be very convenient, because it provides an acceptable calculation time and also stability and simplicity of the computer procedure. This method is a direct generalization of the rotation method (or Jakobi method) [11] for real symmetrical matrices in complex arithmetics. The eigenvectors of the complex symmetrical matrix are mutually orthogonal

$$\sum_{ms} \tilde{B}_{ms}(j)\, \tilde{B}_{ms}(j') = \delta_{jj'} . \tag{2.9}$$

But unlike the Laue case, equation (2.9) does not give the possibility to determine the quantities λ_j in an analytical form because of the complicated character of the set (2.7). Therefore, the set (2.7) has also to be solved numerically. Here, following the two-beam case, it is natural to consider separately the case of an infinitely thick plate (practically $t \gg L_{ex}$, where L_{ex} is the extinction length).

Indeed, the imaginary part of the quantity ε_j, can have any sign and a value as large as $1/L_{ex}$ in the complete reflection region. Therefore, some of the quantities $c_m(j)$ are exponentially large at $t \gg L_{ex}$. In the two-beam case such modes were known to be not excited in a crystal. The analogous situation arises also in the case of multiple diffraction. In the thick crystal only such modes are excited for which $\varepsilon_j'' > 0$ ($\varepsilon = \varepsilon' + i\varepsilon''$). The corresponding coefficients $\lambda(j)$ are defined from the truncated set (2.7) which consists of the equation with multipliers $c_m = 1$. As can be shown, the number of eigenvalues ε_j with negative imaginary part is exactly equal to the double number of Bragg reflecting beams. Consequently, the truncated set has only one solution.

From the experimental point of view the amplitude of the X-ray electric field leaving the crystal is of interest. Let us consider the radiation part going out of the crystal along the $\boldsymbol{k}_m$ direction. If the polarization state of the radiation is s' and one of the incident wave is s, then the field amplitude of this part reads

$$\boldsymbol{E}_m^{s's}(r) = \exp[i\boldsymbol{k}_0\boldsymbol{r}_1 + i\boldsymbol{k}_m(\boldsymbol{r} - \boldsymbol{r}_1)] \left(\frac{\gamma_0}{\gamma_m}\right)^{1/2} \boldsymbol{e}_{ms'} P_m^{s's}(\boldsymbol{q}_0, t)\, A_s , \tag{2.10}$$

$$P_m^{s's}(\boldsymbol{q}_0, t) = \sum_j B_{ms'}(j)\, \lambda_s(j, t)\, D_m(j, t) . \tag{2.11}$$

Here

$$\left.\begin{aligned} \boldsymbol{k}_m &= \boldsymbol{k}_0 + \boldsymbol{h}_m - \alpha_m(\boldsymbol{q}_0)\, \boldsymbol{n}/2 , \\ D_m(j, t) &= \begin{cases} \exp[i(\varepsilon_j + \alpha_m)\, t/2]; & \gamma_m > 0 , \\ 1; & \gamma_m < 0 . \end{cases} \end{aligned}\right\} \tag{2.12}$$

The parameter α_m in (2.12) is determined by (2.6). It arises in the expression for the vacuum wave vector because of the dispersion law $k_m^2 = k_0^2$. Formula (2.10) is valid for the Bragg-reflected beams in the space outside the entrance crystal surface and for the Laue-diffracted beams in that outside the exit surface.

The coefficients of transmission R_0 and reflection R_m, $m \neq 0$, are defined simply in terms of the amplitude $P_m^{s's}$. Let the incident radiation be plane-polarized, for example synchrotron radiation. If φ is the angle between the polarization plane and the vector $\boldsymbol{e}_{0\pi}$ then

$$R_m(\varphi) = \frac{|\gamma_m|}{\gamma_0} \frac{|\boldsymbol{E}_m|^2}{|A|^2} = \bar{R}_m + X_m \cos(2\varphi) + Y_m \sin(2\varphi) , \tag{2.13}$$

where

$$\left.\begin{aligned} \bar{R}_m &= \tfrac{1}{2}\sum_{ss'} |P_m^{ss'}|^2\,, \qquad |A|^2 = \sum_s |A_s|^2\,, \\ X_m &= \bar{R}_m - \sum_s |P_m^{s\sigma}|^2\,, \qquad Y_m = \mathrm{Re}\left\{\sum_s P_m^{s\pi} P_m^{s\sigma *}\right\}. \end{aligned}\right\} \tag{2.14}$$

In the case of unpolarized radiation we have to average (2.13) over the angle φ. As a result, $R_m = \bar{R}_m$.

The dependence of the vector $\boldsymbol{q}_0$ on the three parameter projections is of most interest. These parameters define direction and frequency of the incident beam. However, in the case of the systematic diffraction, the quantities R_m depend effectively on only two parameters. Indeed, due to a nonresonance interaction between X-rays and crystal, we can neglect the slight frequency dependence of the quantities χ_m (see equation (2.5)) in the frequency region corresponding to the Bragg diffraction. Then the matrix G depends on $\boldsymbol{q}_0$ only through the parameter α_m. Let us introduce the unit vector $\boldsymbol{n}_{0R}$ [7] along the direction connecting the centre of a circle described by the reciprocal-lattice-vector polygon and the point 0. After choosing the vector $\boldsymbol{e}_2$ in (2.2) in the reciprocal-lattice-vector plane $\boldsymbol{e}_2 = \boldsymbol{e}_{0\sigma}$, we have

$$\alpha_m = \frac{2}{\gamma_m}\left[(\boldsymbol{h}_m \boldsymbol{n}_{0R})\,\theta + (\boldsymbol{h}_m \boldsymbol{e}_{0\sigma})\,\theta_2\right], \tag{2.15}$$

$$\theta = \theta_1 \cos\theta_0 + \theta_\omega \sin\theta_0\,, \qquad \theta_\omega = (\omega - \omega_0)/\omega_0\,, \tag{2.16}$$

where θ_0 is the angle between $\boldsymbol{s}_0$ and the unit vector $\boldsymbol{n}_h$ of a normal to the reciprocal-lattice-vector plane.

According to (2.16) the change of the incident radiation frequency is compensated by a corresponding change of the beam direction. At small scattering angles ($\theta_0 < \pi/4$) realized in the Laue case, the necessary angular shift does not exceed, as a rule, the relative frequency change. On the contrary, a coplanar diffraction (when $\theta_0 = \pi/2$) is realized easily and is of more interest in the cases of Bragg reflection. In the coplanar case the parameter θ describes purely a frequency dependence, and the dependence on the angle in the plane perpendicular to the reciprocal-lattice-vector plane vanishes in an approximation linear in $\boldsymbol{q}_0$.

3. Concrete Example: The Bragg Reflection of CuK_α Radiation in the Three-Beam (111/11$\bar{1}$) Case in Silicon

We worked out the FORTRAN computer program for the calculation of the coefficient $R_m(\theta, \theta_2, t, \varphi)$ along a scheme described in the previous section. As an example, we consider the three-beam (111/11$\bar{1}$) case of CuK_α radiation diffraction ($\lambda = 1.54$ Å) in a silicon crystal plate with the entrance surface perpendicular to the [1$\bar{1}$0] direction. This case is of interest because it permits an analytical solution of the problem on the $\theta_2 = 0$ line that is situated in the symmetry plane. The solution for the Laue geometry was obtained for the first time in [12, 13]. A generalization to the Bragg reflection case for an infinitely thick crystal is trivial, therefore, we write the final result only. Let the polarization state of the incident beam be standard (π or σ), then

$$R_{1s}(\theta) = R_{2s}(\theta) = \frac{0.5}{|y_s \pm \sqrt{y_s^2 - 1}|^2}, \tag{3.1}$$

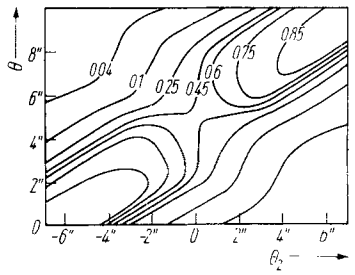

Fig. 1

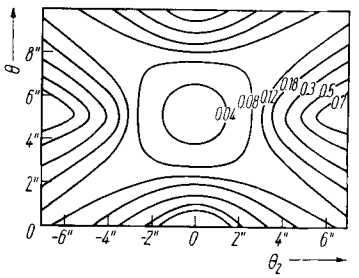

Fig. 2

Fig. 1. The coefficient $\overline{R_1}$ of a reflection of nonpolarized radiation from a thick silicon plate in three-beam (111/11$\bar{1}$) case. The entrance surface is perpendicular to (1$\bar{1}$0)

Fig. 2. The transmission coefficient $\overline{R_0}$ for a plate with at thickness 2 μm and the same experimental conditions as in Fig. 1

where

$$\left.\begin{aligned} y_s &= \frac{\theta - \theta_0}{\theta_{1s}}, \qquad \theta_0 = \frac{2\chi_0}{A}, \qquad \theta_{1s} = -\frac{2\chi_1 C_s}{A}, \\ A &= \frac{2}{\chi_0}(\boldsymbol{h}_1 \boldsymbol{n}_{0R}), \qquad C_s^2 = \begin{cases} 1 + 2(\mathbf{s}_0\mathbf{s}_1)^2 - (\mathbf{s}_1\mathbf{s}_2); & s = \pi, \\ 1 + (\mathbf{s}_1\mathbf{s}_2); & s = \sigma. \end{cases} \end{aligned}\right\} \tag{3.2}$$

Formula (3.1) differs from the corresponding expression for the two-beam reflection coefficient (see, for example, [14]) only by a factor 0.5 and the polarization factor C_s. The real part of the quantity θ_{1s} is easily seen to determine the angular region of total reflection, with θ_{1s} being proportional to C_s. In the present case $C_s^2 \lessapprox 2$, contrary to the two-beam case where $C_s^2 < 1$. Therefore, the three-beam angular region of total reflection along the line $\theta_2 = 0$ is broader than the two-beam one, but the value of the maximum is only 1/2 because of the energy conservation law.

It is easy to understand, taking into account the symmetry of the considered case that the relation $\overline{R}_2(\theta, \theta_2) = \overline{R}_1(\theta, -\theta_2)$ holds. Consequently it is sufficient to consider one of the diffraction beams only. Fig. 1 shows the reflection coefficient $\overline{R}_1(\theta, \theta_2)$ for nonpolarized radiation in the angular region $0 \leqq \theta \leqq 10''$, $-7'' \leqq \theta_2 \leqq 7''$ in the thick crystal. The calculations have been carried out with account of the true absorption of X-rays in the crystal, this fact being the reason for a maximum asymmetry in the two-beam region. As can be seen from the figure, the analytical solution (3.1) on the $\theta_2 = 0$ line does not give the right sense of the three-beam total reflection region which is a gentle pass with a smooth minimum along the two-beam line and with a smooth maximum in the perpendicular direction.

Fig. 2 shows the transmission coefficient $\overline{R}_0(\theta, \theta_2)$ for the same angular region and for a plate with thickness $t = 2$ μm. It follows from the calculation that the extinction length is reduced when penetrating in the many-beam region. The reflection coefficient R_1 for the plate of such a thickness differs slightly from that presented on Fig. 1.

4. Reflection of a Plane Wave at Several Surfaces of the Same Crystal

The calculation of the coefficient of many-beam reflection at several surfaces of the same crystal in the general case is a somewhat more complicated problem. In the present section we restrict our treatment to the general formulation of this problem in a form which is convenient for working out the computer program.

Let the plane wave with the wave vector $\boldsymbol{k}_0$ fall on the first surface of a crystal with the inner normal vector $\boldsymbol{n}_1$. Several beams can go out of the crystal. Let us consider the beam with the wave vector $\boldsymbol{k}_1$ falling on the second surface of the crystal with the inner normal $\boldsymbol{n}_2$ from which, in particular, the beam with the wave vector $\boldsymbol{k}_2$ goes out, and so on. After n reflections the amplitude of the electric field can be written in the form

$$\boldsymbol{E}_n^{s's}(r) = \mathrm{e}^{iq(\boldsymbol{r})}\, \boldsymbol{e}_{ns'} \Gamma P_{12\ldots n}^{s's}(\boldsymbol{q}_0)\, A_s\,, \tag{4.1}$$

where

$$\varphi(r) = \sum_{m=0}^{n} \boldsymbol{k}_m(\boldsymbol{r}_{m+1} - \boldsymbol{r}_m)\,, \qquad \boldsymbol{k}_m = \boldsymbol{\varkappa}_m + \boldsymbol{q}_m\,, \tag{4.2}$$

$$\boldsymbol{q}_m = \boldsymbol{q}_{m-1} - \alpha_m \boldsymbol{n}_m/2\,, \qquad \alpha_m = 2\,\frac{(\boldsymbol{h}_m \boldsymbol{q}_{m-1})}{\varkappa_0 \gamma_{mm}}\,, \tag{4.3}$$

$$\Gamma = \left\{\frac{\gamma_{01}}{\gamma_{11}}\,\frac{\gamma_{12}}{\gamma_{22}} \ldots \frac{\gamma_{n-1.\,n}}{\gamma_{nn}}\right\}^{1/2}, \qquad \gamma_{km} = (\boldsymbol{s}_k \boldsymbol{n}_m)\,, \tag{4.4}$$

$$P_{12\ldots n}^{s's}(\boldsymbol{q}_0) = \sum_{s_1 \ldots s_{n-1}} P_n^{s's_{n-1}}(\boldsymbol{q}_{n-1}) \ldots P_2^{s_2 s_1}(\boldsymbol{q}_1)\, P_1^{s_1 s}(\boldsymbol{q}_0)\,. \tag{4.5}$$

Here $\boldsymbol{h}_m = \boldsymbol{\varkappa}_m - \boldsymbol{\varkappa}_{m-1}$, $\boldsymbol{r}_0$ is the point on the source surface, $\boldsymbol{r}_{n+1} = \boldsymbol{r}$ the detection point, $\boldsymbol{r}_m$ the point on the m-th surface of the crystal.

The vector $\boldsymbol{q}_m$ determines the degree of difference between the vectors $\boldsymbol{k}_m$ and $\boldsymbol{\varkappa}_m$, i.e. in fact the extent to which the Bragg conditions in the m-th reflection is not satisfied. It is essential that only the vector $\boldsymbol{q}_0$ is independent among the vectors $\boldsymbol{q}_m$. The remaining vectors are determined by $\boldsymbol{q}_0$ through (4.3). From the physical point of view formula (4.3) describes the angular divergence change of the incident beam, which arises from the condition of X-ray frequency conservation at reflection. In the approximation linear in $q/\varkappa$ this condition is reduced to the equality $\boldsymbol{\varkappa}_{m-1}\boldsymbol{q}_{m-1} = \boldsymbol{\varkappa}_m \boldsymbol{q}_m$. We note that the vectors $\boldsymbol{\varkappa}_{m-1}$, $\boldsymbol{q}_{m-1}$ at the m-th reflection play the same role as the vectors $\boldsymbol{\varkappa}_0$, $\boldsymbol{q}_0$ play at the first reflection, i.e. one many-beam set of vectors is numbered differently at every reflection.

The amplitude $P^{s's}$, according to (2.15), depends only on the two parameters θ and θ_2. In the case of several reflections, the formulae describing the direct transition from $\theta^{(m-1)}$, $\theta_2^{(m-1)}$ to $\theta^{(m)}$, $\theta_2^{(m)}$ are thought to be useful besides (4.3). Let us introduce the orthonormalized basis $\boldsymbol{n}_{mR}$, $\boldsymbol{e}_{m\sigma}$, $\boldsymbol{n}_h$ tied with point m and mark them for the sake of brevity through $\boldsymbol{a}_s^{(m)}$, $s = 1, 2, 3$. Then

$$\boldsymbol{q}_m = \sum_s \xi_s^{(m)} \boldsymbol{a}_s^{(m)}\,. \tag{4.6}$$

After substitution of (3.6) into (3.3), we have

$$\xi_s^{(m)} = \sum_{s'=1,2} D_m^{ss'} \xi_{s'}^{(m-1)}\,, \tag{4.7}$$

where

$$D_m^{ss'} = (\boldsymbol{a}_s^{(m)} \boldsymbol{a}_{s'}^{(m-1)}) - \frac{1}{\varkappa_0 \gamma_{mm}} (\boldsymbol{a}_s^{(m)} \boldsymbol{n}_m)\, (\boldsymbol{h}_m \boldsymbol{a}_{s'}^{(m-1)})\,. \tag{4.8}$$

The matrix D_m is three-dimensional, but we are interested only in the two-dimensional part with $s, s' = 1, 2$. In this case, (4.7) gives the necessary connection because $\xi_1 = \theta$, $\xi_2 = \theta_2$. Thus the two-dimensional transition matrices can be calculated easily in every concrete case by (4.8). This matrix makes it possible to calculate the two-beam regions of total reflection for all surfaces and to write the diagram analogous to the Du Mond diagram of the theory of two-beam spectrometers [14].

5. Reflection of the Spherical Wave

As it is known, an atom is the source of X-ray radiation, and coherence is preserved only for the radiation of a separate atom. Therefore, the incident-spherical-wave approach is the most natural one for the calculation of interference phenomena. The theory of multiple spherical-wave X-ray diffraction in the Laue case has been formulated in [7]. In this section we present the generalization of this theory to the Bragg reflection case.

Let the radiation of a source placed at the point $\boldsymbol{r}_0$ fall on a crystal. We present the electric field amplitude as a twofold Fourier integral and consider the little angular region near the Bragg direction. Within this angular region the amplitude in the space before the crystal can be written in the form

$$\boldsymbol{E}_s^{(in)}(\boldsymbol{r}, \omega) = \frac{2\pi i}{\varkappa_0} \int \frac{\mathrm{d}\boldsymbol{q}_{0\perp}}{(2\pi)^2} \mathrm{e}^{i\boldsymbol{Q}_0(\boldsymbol{r}-\boldsymbol{r}_0)} \sum_s A_s(\omega)\, \boldsymbol{e}_{0s} , \tag{5.1}$$

where

$$\boldsymbol{Q}_0 = \boldsymbol{k}_0 - \frac{q_{0\perp}^2}{2\varkappa_0} \boldsymbol{s}_0 , \qquad \boldsymbol{q}_{0\perp} = \varkappa_0(\theta_1 \boldsymbol{e}_{0\pi} + \theta_2 \boldsymbol{e}_{0\sigma}) . \tag{5.2}$$

Here we preserve, as in [7], the term quadratic in $\boldsymbol{q}_{0\perp}$ in the wave vector expression, and assume that the amplitude A_s and the polarization vectors $\boldsymbol{e}_{0s}$ do not depend on $\boldsymbol{q}_{0\perp}$. Although the characteristic values of the angles θ_1 and θ_2 are small ($\approx 10^{-5}$), the phase connected with the second-order term is of order $\varkappa_0\theta^2 L$, where L is the source–crystal distance. Consequently, it may be essential when L enlarges. As it has been shown in [6] this term becomes essential when L is equal to ≈ 1 m, a situation that is experimentally achievable.

As a result of the reflection at the first crystal surface the vector $\boldsymbol{Q}_0$ is replaced by $\boldsymbol{Q}_1$. With account of terms to second power in $q/\varkappa$, we have

$$\boldsymbol{Q}_1 = \boldsymbol{k}_1 - \frac{q_{0\perp}^2}{2\varkappa_0} \boldsymbol{s}_0 - \alpha_1^{(2)} \boldsymbol{n}_1/2 , \tag{5.3}$$

where the vector $\boldsymbol{k}_1$ is determined by (4.2), (4.3) and the quantity $\alpha_1^{(2)}$ is determined by formula (8) in [7] which can be written in another form as

$$\alpha_1^{(2)} = C_1 , \qquad C_m = \frac{1}{\varkappa_0 \gamma_{mm}} [q_{0\perp}^2(1 - \boldsymbol{s}_0\boldsymbol{s}_m) + q_m^2 - q_0^2] . \tag{5.4}$$

Considering n reflections consistently, we obtain easily the following expression for $\boldsymbol{Q}_n$:

$$\boldsymbol{Q}_n = \boldsymbol{k}_n - \frac{q_{0\perp}^2}{2\varkappa_0} \boldsymbol{s}_0 - \sum_{m=1}^{n} \alpha_m^{(2)} \boldsymbol{n}_m/2 \tag{5.5}$$

in which the quantity $\alpha_m^{(2)}$ is defined by the recurrence formula

$$\alpha_m^{(2)} = C_m - \sum_{k=1}^{m-1} \alpha_k^{(2)} \frac{\gamma_{mk}}{\gamma_{mm}} . \tag{5.6}$$

We note that the second-order corrections must be considered only where the corresponding vector is multiplied by a long distance of the order of 1 m. Because all the reflecting surfaces belong in our case to the same crystal, the distances between them are small. Therefore, we can replace all $\boldsymbol{Q}_m$, $m = 1, \ldots, n-1$ by $\boldsymbol{k}_m$ with a good accuracy. We can also neglect the second-order terms in α_m when calculating the reflection amplitude and use the formulae (4.3), (4.5). However, these terms must

be considered in $\boldsymbol{Q}_0$, if the source–crystal distance is long, and also in $\boldsymbol{Q}_n$, if there is a long crystal–film distance. Although the formula for $\boldsymbol{Q}_n$ is a rather cumbersome one, in concrete examples considerable simplifications arise.

Considering the above, we can write the amplitude of a field passed through the crystal in the form

$$\boldsymbol{E}_n^{s's}(\boldsymbol{r}, \omega) = \frac{2\pi i}{\varkappa_0} \boldsymbol{e}_{ns'} \int \frac{\mathrm{d}\boldsymbol{q}_{0\perp}}{(2\pi)^2} \Gamma \, \mathrm{e}^{i\varphi(\boldsymbol{q}_0, \boldsymbol{r})} \, P_{12\ldots n}^{s's}(\boldsymbol{q}_0) \, A_s(\omega) \,, \tag{5.7}$$

where

$$\varphi(\boldsymbol{q}_0, \boldsymbol{r}) = \boldsymbol{Q}_0(\boldsymbol{r}_1 - \boldsymbol{r}_0) + \sum_{m=1}^{n-1} \boldsymbol{k}_m(\boldsymbol{r}_{m+1} - \boldsymbol{r}_m) + \boldsymbol{Q}_n(\boldsymbol{r} - \boldsymbol{r}_n) \,. \tag{5.8}$$

If the crystal is cut in such a way that the last surface reflects into the same direction two or more beams which pass on differrent ways (interferometer), then the term $\Gamma \, \mathrm{e}^{i\varphi} \, P$ has to be replaced by the sum of several terms of the same type.

In accordance with the method of geometrical optics, the trajectory of rays is defined from the condition of equality to zero of the terms linear in $\boldsymbol{q}_{0\perp}$ in the phase (5.8). Because the component of $\boldsymbol{q}_m$ parallel $\boldsymbol{\varkappa}_m$ does not depend on $\boldsymbol{q}_{0\perp}$, this condition is satisfied when the vectors $(\boldsymbol{r}_{m+1} - \boldsymbol{r}_m)$ are parallel $\boldsymbol{\varkappa}_m$. The diffraction pattern arises on the plane perpendicular $\boldsymbol{\varkappa}_n$. In the nonpolarized radiation case the intensity of the n-th beam is equal to

$$I_n(\boldsymbol{r}) = \frac{\gamma}{2\pi} \int \frac{\mathrm{d}\theta_\omega}{(\theta_\omega^2 + \gamma^2)} \sum_{ss'} |F_n^{ss'}(\boldsymbol{r}, \theta_\omega)|^2 \,, \tag{5.9}$$

$$F_n^{ss'}(\boldsymbol{r}, \theta_\omega) = \frac{\varkappa_0}{2\pi} \Gamma \int \mathrm{d}\theta_1 \, \mathrm{d}\theta_2 \, \mathrm{e}^{i\varphi} \, P_{12\ldots n}^{ss'}(\boldsymbol{q}_0) \,. \tag{5.10}$$

Here we also take into account the nonmonochromaticity of the radiation which is of order of the natural width of a characteristic line of a X-ray tube spectrum; γ is a relative half-width of the line.

According to (2.15), the amplitude $P^{ss'}$ depends on θ_1 and θ_ω only through a definite combination θ. In the nonplanar case we can proceed to a new variable θ instead θ_1 in (5.10), then the role of θ_ω reduces only to the shift of the whole pattern by some vector proportional θ_ω [7]. In the cases close to coplanar, however, the shift vector becomes very long leading to a strong averaging of the diffraction pattern along the direction of the shift. In the coplanar case, the dependence on the distance along this direction vanishes (in an approximation linear in θ), and the integration over θ_ω needs to be carried out independently. In this case the spectrum characteristics of the reflected radiation, in particular, the coherence length, are determined completely by the diffraction process, not by the source.

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