DYNAMICAL THEORY OF COPLANAR N-BEAM X-RAY DIFFRACTION IN MULTILAYERED STRUCTURES

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A new approach to calculating the coplanar N-beam X-ray dynamical diffraction in multilayered structures has been presented. The theory produces adequate results in the wide range of angles, including the grazing incidence. It can be applied to calculate the reflected beam and diffraction by thick layers. It can also be used to take into account practically any number of reciprocal lattice sites that participate in diffraction.

1. Introduction

Modern electronics develops towards the miniaturization of the characteristic dimensions of integrated microcircuit components. In so doing, not only do the difficulties connected with the creation of such nano-sized structures grow, but also the difficulties associated with the monitoring of their geometry and composition.

One of the basic tools for non-destructive structural analysis is the diffraction of X-rays. Most techniques that are used nowadays for analysis are based on the solution of the corresponding inverse problem in the framework of the kinematic or two-beam dynamical theory. Both theories include a plenty of simplifications and, being applied to the structures with thick layers, in the case of the wide-angle diffraction or the simultaneous diffraction from several sets of crystal planes, and so on, produce incorrect results. Therefore, it is often necessary to apply more correct theories, with a smaller number of simplifications. Moreover, in order to improve the accuracy and to extend the angular range of analysis, wave vectors in the medium should be determined numerically [1].

In this work, we expound the theory of the multiple-beam diffraction of X-rays in layered structures. It is based on works [2, 3] dealing with the multiple-beam diffraction in single-layered structures, and on works [4–6]. The results of the latter were also taken into account while solving the problems with thick layers [4] and in the grazing geometry [7]. Some useful ideas concerning the solution of the dispersion equation have been borrowed from work [8].

Most often considered is the coplanar multiple-beam diffraction of X-rays [2]. That is why just this case is examined in this work. Moreover, such a consideration allows the time of calculations to be reduced by several times, which is especially important in the case of the automated fitting of spectra.

2. Dispersion Equation

In the framework of the dynamical theory, X-rays are regarded as electromagnetic waves. Therefore, assuming that the conductivity of the medium and the influence of its free charges are absent (which is eligible for X-rays [10]), expanding the polarizability of the medium into the series of its Fourier components (χ_{h-p}), and trying the solution of the relevant Maxwell equations in the form of a Bloch wave, we obtain the system of equations for the nonzero strengths $\vec{E}_h$ of the waves in the crystal [10]:

$$\frac{|k_h|^2\vec{E}_h - K^2\vec{E}_h}{K^2} \approx \sum_p \chi_{h-p}\vec{E}_p, \qquad (1)$$

where $K = \frac{\omega}{c} = \frac{2\pi}{\lambda}$ is the length of the wave vector in vacuum, $k = nK$ is the length of the wave vector in the medium with the index of refraction $n \approx \sqrt{1+\chi_0}$.

Let us change over to the dimensionless coordinates

$$\frac{k_h}{K} \to k_h, \quad \frac{h}{K} \to h, \qquad (2)$$

where h is the length of the reciprocal lattice vector.

Taking into account that, in reality, there can be the infinite number of wave fields in the crystal, and N waves of them can turn out strong enough, the wave

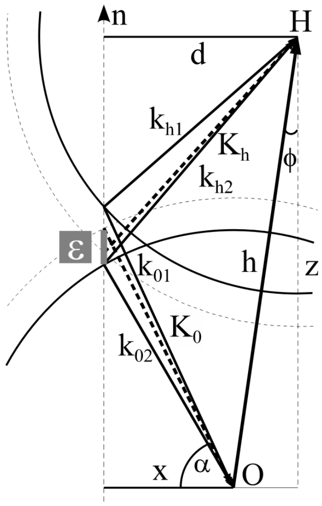

Fig. 1. Dispersion surface in the two-wave case

amplitude at the point which is described by the radius-vector $\vec{r}$ looks like

$$E(\vec{r}) = \sum_{h=0}^{N-1} E_h \exp(i\vec{k}_h\vec{r}).$$

Then, in the coplanar case, Eq. (1) reads

$$(k_h^2 - n^2)E_h = \sum_{p\neq h} \chi_{h-p}E_p. \qquad (3)$$

Equation (3) divided by the amplitude of the incident wave and written down in the matrix form looks like

$$\Delta_E E = 0, \qquad (4)$$

where

$$\Delta_E = \begin{pmatrix} k_0^2 - n^2 & -\chi_{0,-1} & -\chi_{0,-2} & \cdots & -\chi_{0,-(N-1)} \\ -\chi_{1,0} & k_1^2 - n^2 & -\chi_{1,-2} & \cdots & -\chi_{1,-(N-1)} \\ -\chi_{2,0} & -\chi_{2,-1} & k_2^2 - n^2 & \cdots & -\chi_{2,-(N-1)} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ -\chi_{N-1,0} & -\chi_{N-1,-1} & -\chi_{N-1,-2} & \cdots & k_{N-1}^2 - n^2 \end{pmatrix}, \qquad (5)$$

$$E = \begin{pmatrix} 1 \\ c_1 \\ c_2 \\ \cdots \\ c_{N-1} \end{pmatrix}, \qquad (6)$$

and $c_i = E_h^i/E_0^i$ are the coefficients.

In accordance, the dispersion equation in the general case looks like

$$\Delta_E = 0. \qquad (7)$$

It is rather inconvenient to try wave vectors in the form, which they have in Δ_E, because, on finding their lengths, one would have to determine their directions separately. Therefore, let us take advantage of the fact the tangential component of the wave vector keeps its length on the refraction. We introduce the quantity ε which characterizes the difference between the normal components of wave vectors in the medium, k_h, and in vacuum, K (Fig. 1). Then,

$$\vec{k}_h = \vec{K}_0 + \vec{h} + K\varepsilon\vec{n}, \qquad (8)$$

where $\vec{h}$ is the corresponding diffraction vector, $\vec{K}_0$ is the wave vector of the incident wave, and $\vec{n}$ is the vector of the normal. It is evident that, if the wave field equals zero, $\vec{h} = 0$ and $\vec{k}_0 = \vec{K}_0 + K\varepsilon$. Using the notation introduced and taking into account normalization (2) that was adopted above, we obtain

$$k_h^2 = \left(\vec{S}_0 + \vec{h} + \varepsilon\vec{n}\right)\left(\vec{S}_0 + \vec{h} + \varepsilon\vec{n}\right) =$$

$$= 1 + 2\left(\vec{S}_0 \cdot \vec{h}\right) + 2\varepsilon\left(\vec{S}_0 \cdot \vec{n}\right) + 2\varepsilon\left(\vec{h} \cdot \vec{n}\right) + h^2 + \varepsilon^2, \qquad (9)$$

where $\vec{S}_0$ is a unit vector directed along $\vec{K}_0$: $\vec{S}_0 \equiv \vec{K}_0/K$. It is obvious that

$$\left(\vec{S}_0 \cdot \vec{n}\right) = \cos(90^\circ + \alpha) = -\sin\alpha,$$

$$\left(\vec{S}_0 \cdot \vec{h}\right) = h\cos(\alpha + 90^\circ - \varphi) = -h\sin(\alpha - \varphi),$$

$$\left(\vec{h} \cdot \vec{n}\right) = h\cos\varphi,$$

where α is the angle between the incident beam and the surface, and φ is the angle between the vector $\vec{h}$ and a normal to the surface. Therefore,

$$k_0^2 = \varepsilon^2 + 1 - 2\varepsilon\sin\alpha,$$

$$k_h^2 = \varepsilon^2 + 1 + h^2 - 2\varepsilon \sin\alpha - 2h \sin(\alpha - \varphi) + 2\varepsilon h \cos\varphi.$$

The sought quantities are

$$k_0^2 - n^2 = \varepsilon^2 - 2\sin\alpha \cdot \varepsilon + \left(1 - n^2\right),$$

$$k_h^2 - n^2 = \varepsilon^2 + 2\left(h\cos\varphi - \sin\alpha\right)\varepsilon + \left(1 - n^2\right) + h\left(h - 2\sin(\alpha - \varphi)\right).$$

Then, the dispersion equation (7) reads

$$\Delta_E = \varepsilon^2 \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix} + \varepsilon \begin{pmatrix} -2\sin\alpha & 0 & \cdots & 0 \\ 0 & 2\left(h_1\cos\varphi_1 - \sin\alpha\right) & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 2\left(h_1\cos\varphi_1 - \sin\alpha\right) \end{pmatrix} +$$
$$+ \begin{pmatrix} 1 - n^2 & -\chi_{0,-1} & \cdots & -\chi_{0,-(N-1)} \\ -\chi_{1,0} & 1 - n^2 + h_1\left(h_1 - 2\sin(\alpha - \varphi_1)\right) & \cdots & -\chi_{1,-(N-1)} \\ -\chi_{2,0} & -\chi_{2,-1} & \cdots & -\chi_{2,-(N-1)} \\ \cdots & \cdots & \cdots & \cdots \\ -\chi_{N-1,0} & -\chi_{N-1,-1} & \cdots & 1 - n^2 + h_N\left(h_N - 2\sin(\alpha - \varphi_N)\right) \end{pmatrix} = 0. \tag{10}$$

In the matrix notation,

$$\Delta_E = \varepsilon^2 I + \varepsilon A + B, \tag{11}$$

where I is the identity matrix, while A and B are the corresponding matrices from Eq. (10):

$$A = \left\{\delta_{ij} \cdot 2\left(h_i\cos\varphi_i - \sin\alpha\right)\right\},$$

$$B = \begin{cases} i = j: & 1 - n^2 + h_i\left(h_i - 2\sin(\alpha - \varphi_i)\right), \\ i \neq j: & -\chi_{i,-j}, \end{cases}$$

$j, i = 0, \ldots, N-1$, $h_0 \equiv 0$, $\varphi_0 \equiv 0$, and δ_{ij} — delta function.

Substituting Eq. (11) into Eq. (4), we obtain the expression

$$\varepsilon^2 IE + \varepsilon AE = \varepsilon\left(\varepsilon IE + AE\right) = -BE, \tag{12}$$

which, after introducing the notation

$$\varepsilon IE \equiv E_S, \tag{13}$$

looks like

$$\varepsilon\left(E_S + AE\right) = -BE. \tag{14}$$

Combining Eqs. (13) and (14), we obtain

$$\begin{pmatrix} -B & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} D \\ D_S \end{pmatrix} = \varepsilon \begin{pmatrix} A & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} D \\ D_S \end{pmatrix}. \tag{15}$$

Equation (15) comprises the generalized problem to find the eigenvalues ε and is solved with the help of standard algorithms (for example, using the routines that are included into the NAG or IMSL libraries, or the programs presented at the site http://www.srcc.msu.su).

The solutions of this equation are $2N$ eigenvalues ε and $N \times 2N$ eigenvectors that are the wave amplitudes of all the wave fields. Nevertheless, those wave vectors must be normalized by dividing each of N columns by the first value in the column, which is the amplitude of the incident wave and should be reduced to unity. Afterwards, one has to determine $N \times 2N$ normal components of the wave vectors:

$$k_{hz} = \left(\vec{k}_h \cdot -\vec{n}\right) = \sin\alpha - \varepsilon - h_i\cos\varphi_i. \tag{16}$$

Thus, the problem of determining the wave fields in the given substance becomes resolved. Now, let us find the exact values of the wave fields and expand this problem onto the structure that consists of M plane-parallel layers (a superlattice). For this purpose, we must determine the proper boundary conditions.

3. Application of Boundary Conditions

The boundary conditions for electromagnetic waves are the continuity of the tangential (parallel to the surface) components of the electric, $\vec{E}$, and magnetic, $\vec{H}$, fields.

This formulation gives the following equations at each interface [9]:

$$\sum_{n=0}^{2N-1} c_n E_{0n} = \text{const},$$

$$\sum_{n=0}^{2N-1} c_n k_{zn} E_{0n} = \text{const}, \tag{17}$$

where c_n are the coefficients to find, and k_{zn} are the normal components of the wave vectors.

Conditions (17), where the attenuation of the wave owing to its absorption in the layer is taken into account, give

$$S_m F_m E_m = S_{m+1} E_{m+1} \tag{18}$$

for the interface, where E_m is the column vector of strength amplitudes in the m-th layer,

$$S_m = \begin{pmatrix} c_{0,0} & c_{0,1} & \cdots & c_{0\,,2N-1} \\ c_{1,0} & c_{1,1} & \cdots & c_{1\,,2N-1} \\ \cdots & \cdots & \cdots & \cdots \\ c_{N-1,0} & c_{N-1\,,1} & \cdots & c_{N-1\,,2N-1} \\ c_{0,0}k_{z\,0\,,0} & c_{0,1}k_{z\,0\,,1} & \cdots & c_{0\,,2N-1}k_{z\,0,\,2N-1} \\ c_{1,0}k_{z\,1\,,0} & c_{1,1}k_{z\,1,\,1} & \cdots & c_{1\,,2N-1}k_{z\,1,\,2N-1} \\ \cdots & \cdots & \cdots & \cdots \\ c_{N-1,\,0}k_{z\,N-1,\,0} & c_{N-1,\,1}k_{z\,N-1,\,1} & \cdots & c_{N-1\,,2N-1}k_{z\,N-1,\,2N-1} \end{pmatrix}, \tag{19}$$

and

$$F_m = \delta_{i\,j} \exp\left(-ik_{0z}^{j} K t_m\right). \tag{20}$$

t_m is the thickness of the m-th layer, and k_{0z}^{j} stands for $2N$ solutions of the dispersion equation (the first row of the matrix k_z) which correspond to the incident wave.

In order to find the values of the wave amplitudes in the whole structure, we have to solve the matrix equation

$$E_0' = S_0^{-1} S_1 F_1 S_1^{-1} S_2 F_2 \cdots S_{M-1}^{-1} S_M \Phi_M^{(U)} E_M, \tag{21}$$

where M is the number of layers (subscript 0 corresponds to air, M to the substrate), $\Phi_m^{(U,L)} = \delta_{ij} \exp\left(ik_{0z}^{j} K z_m^{(U,L)}\right)$, $z_m^{(U,L)}$ is the distance between the top (U) and the bottom (L) surfaces of the m-th layer, E_0' is the strength amplitude in air, S_0 is the matrix of boundary conditions on the structure surface which equals

$$S_0 = \begin{pmatrix} 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & 0 & 1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 1 \\ K_{z\,0} & 0 & \cdots & 0 & -K_{z\,0} & 0 & \cdots & 0 \\ 0 & K_{z\,1} & \cdots & 0 & 0 & -K_{z\,1} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & K_{z\,N} & 0 & 0 & \cdots & -K_{z\,N} \end{pmatrix}, \tag{22}$$

in the Bragg case,

$$E'_0 = \begin{pmatrix} E_0 \\ 0 \\ 0 \\ E_R \\ E_1 \\ E_{N-1} \end{pmatrix}, \tag{23}$$

E_0 is the amplitude of the incident wave (usually, it is accepted equal to unity), E_R is the amplitude of the wave reflected from the surface; $E_1, \ldots, E_{N-1}$ are the amplitudes of the diffracted waves, $K_{z\,0} \equiv \gamma_0 = \sin\alpha$, and $K_{z\,h} \equiv -\gamma_h = \sqrt{1-(\cos\alpha - h\sin\varphi)^2}$.

The solutions of Eq. (21), obtained in the grazing geometry or for thick layers, are characterized by large errors, because the matrix F_m includes the equal numbers of increasing and decreasing exponents (a half of the dispersion equation roots has negative imaginary parts, and the other half has positive ones). Therefore, we resort to the technique that was proposed in work [5].

First, let us sort the roots of the dispersion equation in the descending order of their imaginary parts, i.e. over the first rows of the corresponding matrices C_n and k_z. Secondly, let us carry out the renormalization

$$E_m \equiv \Phi_m^L E_m, \tag{24}$$

where Φ_m^L is the wave phase on the bottom interface of the m-th layer. At last, let us introduce the matrix

$$X_m = \begin{pmatrix} X^{tt} & X^{tr} \\ X^{rt} & X^{rr} \end{pmatrix} = S_{m-1}^{-1} S_m. \tag{25}$$

into consideration. Then, Eq. (18) can be written down as

$$E_m = X_{m+1} F_{m+1} E_{m+1}. \tag{26}$$

Taking the sorting of the roots described above into account, the first N elements of the matrix E_m represent incident waves, and the other N elements correspond to reflected or diffracted waves, i.e. $E_m = \begin{pmatrix} T_m \\ R_m \end{pmatrix}$ For example, for air, $T_0 = (E_0\ 0\ 0 \ldots 0)$ and $R_0 = (E_R\ E_1\ E_2 \ldots E_{N-1})$. Then, Eq. (26) looks like

$$\begin{pmatrix} T_m \\ R_m \end{pmatrix} = \begin{pmatrix} X^{tt} & X^{tr} \\ X^{rt} & X^{rr} \end{pmatrix} \begin{pmatrix} F_+ & 0 \\ 0 & F_- \end{pmatrix} \begin{pmatrix} T_{m+1} \\ R_{m+1} \end{pmatrix}, \tag{27}$$

where F_+ and F_- are the diagonal $N \times N$-matrices of form (20) which include either increasing or decreasing exponents, respectively.

Furthermore, let us introduce the matrices

$$M^{tt} = (F_+)^{-1} \left(X^{tt}\right)^{-1},$$

$$M^{tr} = -M^{tt} X^{tr} F_-,$$

$$M^{tr} = X^{rt} (X^{tt})^{-1},$$

$$M^{rr} = (X^{rr} - M^{rt} X^{tr}) F_- \tag{28}$$

and rewrite Eq. (27) in the form

$$\begin{pmatrix} T_{m+1} \\ R_m \end{pmatrix} = \begin{pmatrix} M^{tt} & M^{tr} \\ M^{rt} & M^{rr} \end{pmatrix} \cdot \begin{pmatrix} T_m \\ R_{m+1} \end{pmatrix}. \tag{29}$$

Having introduced the matrices

$$W_m^{tt} = A_m W_{m-1}^{tt},$$

$$W_m^{tr} = M_m^{tr} + A_m W_{m-1}^{tr} M_m^{rr},$$

$$W_m^{rt} = W_m^{rt} + B_m M_m^{rt} W_{m-1}^{tt},$$

$$W_m^{rr} = B_m M_m^{rr},$$

$$A_m = M_m^{tt} \left(1 - W_{m-1}^{tr} M_m^{rt}\right)^{-1},$$

$$B_m = W_{m-1}^{rr} \left(1 - M_m^{rt} W_{m-1}^{rt}\right)^{-1}, \tag{30}$$

we obtain

$$\begin{pmatrix} T_m \\ R_0 \end{pmatrix} = \begin{pmatrix} W^{tt} & W^{tr} \\ W^{rt} & W^{rr} \end{pmatrix} \cdot \begin{pmatrix} T_0 \\ R_m \end{pmatrix}. \tag{31}$$

As a result, the reflection from the crystal is described by the matrix equation

$$R_0 = W_M^{rt} T_0. \tag{32}$$

4. Solution Routine

In order to calculate the intensities of X-waves diffracted by a multilayered structure, one has to execute the following actions:

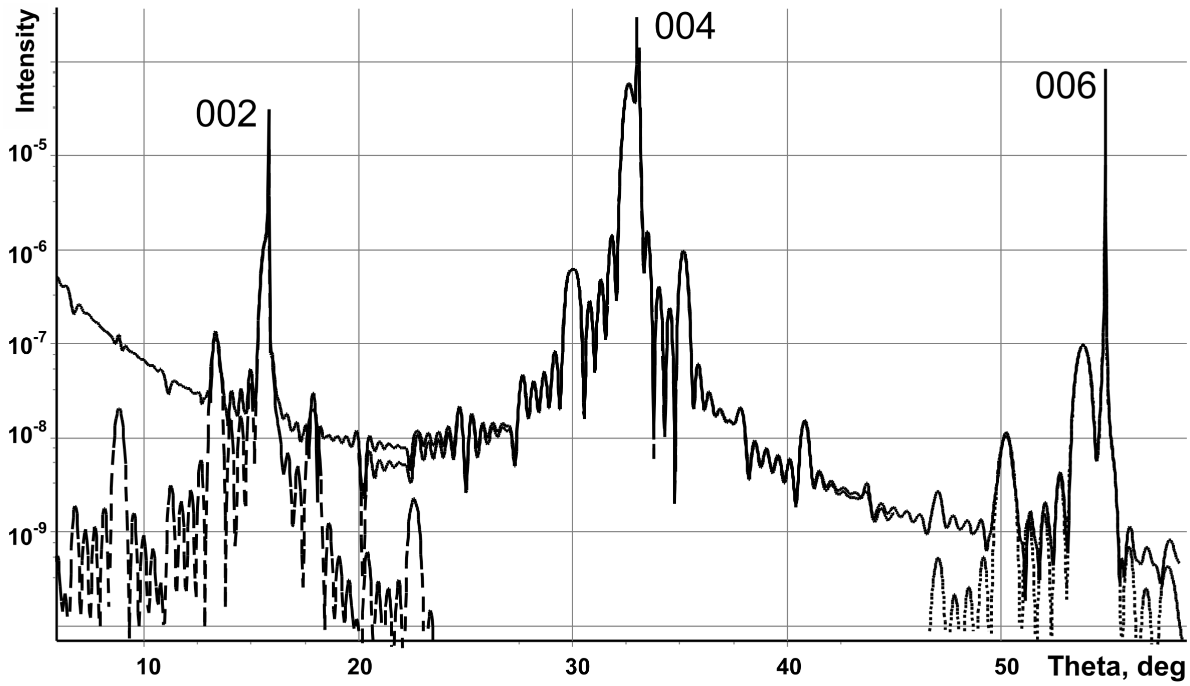

Fig. 2. Example of the wide-angle diffraction by a superlattice (reflexes 200, 400, and 600, from left to right). The solid curve was obtained in the framework of the multiple-beam theory and taking the reflected beam into account. The dotted curves depicted the results of the ordinary two-beam theory

1) Knowing the matrix S_{m-1} for the previous layer, find S_{m-1}^{-1} (for air, S_0 is given by Eq. (22)),

2) Solve the dispersion equation (16), find the matrices k_{hz} and c_n for the m-th layer and sort its rows on the descending of imaginary part of k_{hz},

3) Construct the matrix S_m,

4) Find $X_m = S_{m-1}^{-1} S_m$,

5) Construct the matrix F_- for the first N roots and the matrix F_+^{-1} for the rest,

6) Calculate the matrices M_m,

7) Recursively, find W_m. For air, $W_0^{tt} = I$, $W_0^{rr} = I$, $W_0^{rt} = 0$, and $W_0^{tr} = 0$. For the first layer, $W_1^{tt} = M_1^{tt}$, $W_1^{tr} = M_1^{tr}$, $W_1^{rt} = M_1^{rt}$, and $W_1^{rr} = M_1^{rr}$,

8) Find the coefficient of diffraction from the structure under investigation

$$R_0 = \begin{pmatrix} E_R \\ E_1 \\ E_2 \\ \cdots \\ E_{N-1} \end{pmatrix} = W_N^{rt} \cdot \begin{pmatrix} E_0 \\ 0 \\ 0 \\ \cdots \\ 0 \end{pmatrix},$$

i.e. $E_R = W_N^{rt}[0]\,[0]$, and $E_{hi} = W[i+1]\,[0]$,

9) Find the intensity $\Re = \frac{|\gamma_h|}{\gamma_0} |R|^2$,

10) Obtain the dependence of the intensity on the angle of incidence.

In Fig. 2, the so-called wide-angle diffraction of X-rays by a layered structure is depicted. Four sites of the reciprocal lattice — 000, 002, 004, and 006 — are assumed to take part in diffraction.

5. Conclusions

The dynamical theory of the interaction of X-waves with a substance has been developed in the case where several sites of the reciprocal lattice take part simultaneously in the formation of a diffraction pattern. The theory proposed differs from the theories developed earlier in the following items:

— our variant leads to the correct interpretation of experimental data obtained in the grazing geometry;

— the problem of exponents that infinitely increase in a certain angular range has been resolved;

— in the course of solving the dispersion equation, a new variable was introduced; this variable allows the errors that arise while calculating the diffraction from a large number of reciprocal lattice sites to be avoided;

— the dimensions of the matrices which describe the boundary conditions became lower; this results in the increased rate of calculations;

— the solution is extended onto the angular range far from the exact Bragg position;
— the problem was solved with a minimal number of simplifications, namely, the plane-wave approximation for waves which transmit through the crystal, coplanar geometry, and σ-polarized radiation.

In the nearest future, the theory of the multiple-beam diffraction in layered structures will be extended onto a non-coplanar geometry and an arbitrary polarization state based on the work [10].

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КОМПЛАНАРНА БАГАТОПРОМЕНЕВА ДИНАМІЧНА ТЕОРІЯ ДИФРАКЦІЇ X-ПРОМЕНІВ У ШАРУВАТИХ СТРУКТУРАХ

О.М. Єфанов, В.П. Кладько, В.Ф. Мачулін

Р е з ю м е

Розвинено компланарну теорію динамічної дифракції X-променів у багатошарових структурах для N сильних хвиль. Теорія адекватна для широких кутових діапазонів, ковзної геометрії, розрахунку відбитого променя, для будь-якої товщини шарів і практично будь-якої кількості точок оберненого простору, що беруть участь у дифракції.