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# Covariant Dynamical Theory of X-Ray Diffraction

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## Abstract

The proposed nonstandard diffraction theory is constructed directly from the Maxwell equations for the crystalline medium in the X-ray wavelength range. Analysis of Maxwell's equations for dynamic diffraction is possible using the method of multiple scales which is modified to the vector character of the problem. In this case, the small parameter of the expansion is the Fourier component of the polarizability of the crystal. The second-order wave equation is analyzed without any assumptions about the possibility of the interaction between the refracted and scattered waves which automatically leads to the dynamic character of the scattering. The unified consideration of different geometrical schemes of diffraction including grazing geometry is possible. This is due to the construction of a unified wave field in the crystal and obtaining the field amplitudes according to the boundary conditions. The proposed theory allows generalization to the case of an imperfect crystal. Thus, a unified approach to account for deformations and other crystal structure disturbances in all diffraction schemes is implemented. The determination of a unified wave field without separation of the refracted and scattered waves is of the greatest importance in the analysis of secondary processes.

**Keywords:** X-ray diffraction, dynamic theory, imperfect crystal, perturbation theory, the method of multiple scales, deformation, extinction length, boundary conditions, reflection coefficient

## 1. Introduction

It is possible to separate several fundamental approaches in the theory of dynamical X-ray scattering in the crystal [1, 2].

The Darwin theory [1] is based on the Bragg model for the crystal considered as a family of parallel crystal planes. The X-ray wave reflection is considered as a result of successive transmission and multiple reflections from planes. In this case determination of the diffracted wave amplitude is reduced to the solution of recurrent relations between the amplitudes of transmitted and scattered waves in passing through the specified atomic plane. In essence, the Darwin theory represents a direct extrapolation of the optical task of propagation of light in a layer continuum to the case of wavelengths of the X-ray range.

The Evald-Laue theory [2] was the next stage in the development of theoretical approximations about the character of X-ray wave propagation in the crystal under dynamic scattering. The model approximations of the X-ray crystal interaction were formulated in the framework of this theory, meaning that the X-ray wavelength is comparable to the interatomic distances.

Therefore, the standard continual approximation for electrodynamics of continua proves to be unacceptable, and the scattering from individual charges should be taken into consideration. As is known, taking this into account results in the formalism of 3D periodic dielectric permeability  $\epsilon(\mathbf{r})$  or polarizability  $\chi(\mathbf{r})$  with the lattice spacings of the crystal. The Evald-Laue theory proceeds from the conception of a uniform wave field that appears in the crystal under dynamic scattering. In the two-wave approximation, the wave field is a superposition of refracted and diffracted waves. The determination of field amplitudes is reduced to the solution of a certain dispersion equation following from the fundamental equations of the theory.

In spite of a series of unconditional advantages in the interpretation and theoretical prediction of experimental results on dynamic X-ray scattering in crystals, both the Evald-Laue theory and, substantially, the Darwin theory have the principal limitation that they describe the dynamical diffraction in perfect crystals only.

The necessity of taking into accounts the different deviations from ideal periodicity in the crystal and, first of all, deformations resulted in the creation of the generalized theory developed by Takagi and Taupin [2]. This is based on the approximation of a wave field in the form of superposition of the transmitted and diffracted waves with slowly varied amplitudes depending on the coordinates that leads to the Takagi-Taupin equations to the system of differential equations relative to the field amplitudes. This formalism gives the possibility to describe the dynamical diffraction in a distorted crystal since the distortions of ideal periodicity can be taken into account in the explicit form in the wave field approximation. Correspondingly, the Takagi-Taupin equations become the system of differential equations with variable coefficients.

It is important that the Takagi-Taupin system is shortened and the coordinate second derivatives of field amplitudes are neglected in it. On the one hand, this significantly facilitates the theoretical consideration and makes observable the solution of a series of diffraction problems in standard diffraction geometries when this simplification proves to be justified. On the other hand, the Takagi-Taupin equations become inapplicable under the conditions, for example, of grazing diffraction geometry; then, it is necessary to solve the third- or even fourth-order differential equations [3].

The principal disadvantage of the procedure of equation shortening is related to the impossibility to state correctly the boundary conditions at the crystal-vacuum interface for field amplitudes. Instead of the known classical continuity conditions for tangential components of electric and magnetic fields, the boundary conditions of the type of setting of the normal components of field amplitudes on the crystal surface become vaguely clear but not in line with the Maxwell equations. Of course the solutions of these boundary problems prove to be applicable only for rather large (more correctly significantly exceeding the angle of full external reflection) angles of radiation incidence and yield.

As a result the theory faces the difficulties related to the necessity to solve the third- or fourth-order equations which become virtually overwhelming for the case of the crystal with lattice deformation when the diffraction schemes of the type of sliding diffraction are considered.

At the same time, the Maxwell equations are the first-order equations or the second-order ones in the case of a single wave equation when passing, for example, to an electric field. Namely, this structure of equations agrees with the mentioned classical boundary conditions. This means that the requirement of taking correctly into account the boundary conditions in any theoretical diffraction scheme leads virtually unambiguously to the known structure of wave equation following from the Maxwell equation.

Thus, to overcome the aforementioned difficulties, it is necessary to create the theory directly based on the Maxwell equations using model approximations of crystal polarizability in the X-ray wavelength range.

## 2. A covariant dynamical theory of X-ray scattering in perfect crystals

In this section we follow the original papers [4–7].

### 2.1 Physical diffraction model and basic equation

The model approximations for crystal and X-rays propagating in it are reduced to the following.

The plane monochromatic wave falls from vacuum onto the crystal. The crystal-vacuum interface is considered as a geometrical one so that the classical boundary conditions for optics prove to be applicable. The uniform wave field in the crystal is described by the fundamental Maxwell equations supplemented by the constitutive equation  $\mathbf{D} = \varepsilon(\mathbf{r})\mathbf{E}$  with 3D periodic dielectric permeability  $\varepsilon(\mathbf{r})$  or polarizability  $\chi(\mathbf{r})$  with the lattice spacing. Thereby, the linearity and isotropy of continuum in the X-ray wavelength range and the locality of connection between  $\mathbf{D}$  and  $\mathbf{E}$  are suggested. The possible time dependence is not taken into account; therefore, the possibility of incoherent (in the sense of the change in the radiation frequency) scattering is eliminated. As is seen, the indicated suggestions properly correspond to the model underlying the Ewald-Laue theory if the functional form  $\varepsilon(\mathbf{r})$  is not specified.

The Maxwell equations, as the equations of electromagnetic waves in dielectric, when dispersion is absent, can be written in the form (designations here and below are standard):

$$\text{rot}\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{H}}{\partial t}; \quad (1)$$

$$\text{div}\mathbf{H} = 0; \quad (2)$$

$$\text{rot}\mathbf{H} = \frac{1}{c}\frac{\partial\mathbf{D}}{\partial t} = \frac{1}{c}\frac{\partial}{\partial t}(1 + \chi(\mathbf{r}'))\mathbf{E} = \frac{1}{c}(1 + \chi(\mathbf{r}'))\frac{\partial\mathbf{E}}{\partial t}; \quad (3)$$

$$\text{div}\mathbf{D} = 0 \quad (4)$$

These equations are supplemented by the constitutive relations:

$$\mathbf{D} = \varepsilon(\mathbf{r}')\mathbf{E} = (1 + \chi(\mathbf{r}'))\mathbf{E}; \quad \mathbf{B} = \mu\mathbf{H} = \mathbf{H} \quad (5)$$

As usual, we will consider that the time dependence of  $\mathbf{E}$  and  $\mathbf{H}$  is harmonic:

$$\mathbf{E}(\mathbf{r}', t) = \mathbf{E}(\mathbf{r}') \exp(-i2\pi\nu t); \quad \mathbf{H}(\mathbf{r}', t) = \mathbf{H}(\mathbf{r}') \exp(-i2\pi\nu t).$$

We have the system

$$\begin{aligned} \text{rot}\mathbf{E} &= -\frac{1}{c}\frac{\partial\mathbf{H}}{\partial t} = ik\mathbf{H}; \\ \text{rot}\mathbf{H} &= \frac{1}{c}(1 + \chi(\mathbf{r}'))\frac{\partial\mathbf{E}}{\partial t} = -ik(1 + \chi(\mathbf{r}'))\mathbf{E}. \end{aligned} \quad (6)$$

For economy we use here and below factor  $2\pi$  into  $k$ ,  $2\pi k \rightarrow k$ . We come from system (6) to the basic equation in the standard way:

$$\text{rotrot}\mathbf{E} - k^2(1 + \chi(\mathbf{r}'))\mathbf{E} = 0. \quad (7)$$

In the present section, we will consider the case of a perfect crystal. This will allow us to compare the conclusions of the proposed formalism to the known theoretical results.

We choose the crystal model  $\chi(\mathbf{r}')$  in the form

$$\chi(\mathbf{r}') = \chi_0 + \chi_H \exp(i2\pi\mathbf{H}\mathbf{r}') + \chi_{\bar{H}} \exp(-i2\pi\mathbf{H}\mathbf{r}'). \quad (8)$$

Below, we will bring  $2\pi$  into  $\mathbf{H}$  as for  $k$ ,  $2\pi\mathbf{H} \rightarrow \mathbf{H}$ . Then, we have for Eq. (7)

$$\text{rotrot}\mathbf{E}(\mathbf{r}') - k^2(1 + \chi_0 + \chi_H \exp(i\mathbf{H}\mathbf{r}') + \chi_{\bar{H}} \exp(-i\mathbf{H}\mathbf{r}'))\mathbf{E}(\mathbf{r}') = 0. \quad (9)$$

To take correctly into account the contribution of different terms into Eq. (9) when using the methods of perturbation theory, it is necessary to bring it to the dimensionless form. This procedure assumes the choice of a certain characteristic spatial scale of the problem. Apparently, this is the parameter determining the reciprocal lattice in our problem, namely, the modulus of the reciprocal lattice vector:

$$\frac{\mathbf{H}}{H} = \mathbf{h}; \quad \mathbf{H}\mathbf{r}' = \mathbf{h}\mathbf{r}; \quad \mathbf{r} = \mathbf{H}\mathbf{r}'.$$

$$\text{rotrot}\mathbf{E}(\mathbf{r}) - \kappa^2(1 + \chi_0 + \chi_H \exp(i\mathbf{h}\mathbf{r}) + \chi_{\bar{H}} \exp(-i\mathbf{h}\mathbf{r}))\mathbf{E}(\mathbf{r}) = 0; \quad (10)$$

$$\kappa = \frac{k}{H}.$$

Eq. (10) cannot be exactly solved. Correspondingly, it is necessary to use some method of approximate solution. There are two main ways to analyze Eq. (10). In the first case, taking into account that  $\chi(\mathbf{r}') \ll 1$  Eq. (10) is presented in the form of an inhomogeneous equation, the right side of which is considered as a small perturbation specifying the field of the incident wave:

$$\text{rotrot}\mathbf{E}(\mathbf{r}') - \kappa^2\mathbf{E}(\mathbf{r}') = \chi(\mathbf{r}')\mathbf{E}(\mathbf{r}').$$

The approximate solution is searched in the space beyond the scattering crystal at large distances from it in the form of the first term of a series of the Born expansion. The applicability of this approach is limited by the smallness of the scattering cross section as compared to the geometrical area of the crystal section. As is known this approach results in the kinematical theory [8].

In the second case, two variants of the dynamical theory are developed from Eq. (10). For the first variant, the solution of Eq. (10) is sought in the form of Bloch wave represented in the form of an infinite series of plane waves with wave vectors corresponding to the refracted wave and diffracted waves in the crystal. This Bloch wave is interpreted as a multiwave solution of the dynamical theory. As a result, the use of expansion of  $\chi(\mathbf{r}')$  in a Fourier series leads to an infinite system of the fundamental equations of the algebraic Evald-Laue type.

Since it is not possible to solve an infinite system, one has to be limited as a rule by two equations, that is, by the two-wave approximation.

For the second variant of the theory, the solution of Eq. (10) is presented in the form of plane waves with the slowly varying amplitude. As a result of the two-wave approximation, we obtain the Takagi-Taupin equations which can be interpreted as the recurrent Darwin relations written in the differential form [2].

We propose here to use a new approach to the analysis of Eq. (10). The physical justification of the proposed method indicates the choice of the perturbation parameter and is as follows. The propagation of an X-ray wave in the crystal



unaccompanied by the appearance of diffracted beams is adequately described by the uniform wave equation with  $\varepsilon = 1 + \chi_0$ . This corresponds to the propagation of an X-ray wave in the crystal as a continuum with the refraction factor with respect to the usual laws of optics. This situation can be considered typical. On the contrary the appearance of diffracted beams requires that the definite geometrical conditions be fulfilled for the wave vectors and reciprocal lattice vector. Apparently,  $\chi_H$  is responsible for this cardinal change in the picture of a wave field in the crystal.

Thus, in spite of the fact that all quantities  $\chi_0, \chi_H, \chi_{\bar{H}} \sim 10^{-5} \div 10^{-6}$ , namely,  $\chi_H$ , should be chosen as the perturbation parameter.

## 2.2 Direct expansion and geometric diffraction conditions

We use the simplest perturbation method, direct expansion, in  $\chi_H$ :

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \chi_H \mathbf{E}_1(\mathbf{r}) + \chi_H^2 \mathbf{E}_2(\mathbf{r}) + \dots$$

We will restrict ourselves to the first-order expansion. We have

$$\begin{aligned} & \text{rotrot} \mathbf{E}_0 + \chi_H \text{rotrot} \mathbf{E}_1 + \dots \\ & - \left( \kappa^2 (1 + \chi_0) + \kappa^2 \chi_H \left( \exp(i\mathbf{h}\mathbf{r}) + \frac{\chi_{\bar{H}}}{\chi_H} \exp(-i\mathbf{h}\mathbf{r}) \right) \right) (\mathbf{E}_0 + \chi_H \mathbf{E}_1 + \dots) = 0 \end{aligned} \quad (11)$$

The zeroth approximation corresponds to zero power of the perturbation parameter  $\chi_H$ :

$$\begin{aligned} \text{rotrot} \mathbf{E}_0 - \kappa_0^2 \mathbf{E}_0 &= 0; \\ \kappa_0^2 &= \kappa^2 (1 + \chi_0). \end{aligned}$$

We select the solution of this vector wave equation in the form of superposition of two plane waves:

$$\begin{aligned} \mathbf{E}_0(\mathbf{r}) &= \mathbf{E}_{01}(\mathbf{r}) \exp(i\mathbf{\kappa}_0 \mathbf{r}) + \mathbf{E}_{02}(\mathbf{r}) \exp(-i\mathbf{\kappa}_0 \mathbf{r}); \\ (\mathbf{\kappa}_0 \mathbf{E}_i) &= 0 \end{aligned}$$

The reasons for this selection are the following. The zeroth approximation corresponds to the propagation of two plane transverse waves in opposite directions in the continuum with  $\chi = \text{const}$ . This is a singular analog of the total field in the crystal for the case of an empty lattice. The propagation directions and the wave amplitudes remain indeterminate and are specified below by the boundary conditions at the vacuum-crystal interface.

The first approximation is obtained when all terms in Eq. (11) proportional to the first power of  $\chi_H$  are zero:

$$\begin{aligned} \text{rotrot} \mathbf{E}_1 - \kappa_0^2 \mathbf{E}_1 &= \kappa^2 \left( \exp(i\mathbf{h}\mathbf{r}) + \frac{\chi_{\bar{H}}}{\chi_H} \exp(-i\mathbf{h}\mathbf{r}) \right) \mathbf{E}_0 \\ &= \kappa^2 \left( \exp(i(\mathbf{\kappa}_0 + \mathbf{h})\mathbf{r}) + \frac{\chi_{\bar{H}}}{\chi_H} \exp(i(\mathbf{\kappa}_0 - \mathbf{h})\mathbf{r}) \right) \mathbf{E}_{01} + \dots \quad (12) \\ &+ \kappa^2 \left( \exp(-i(\mathbf{\kappa}_0 - \mathbf{h})\mathbf{r}) + \frac{\chi_{\bar{H}}}{\chi_H} \exp(-i(\mathbf{\kappa}_0 + \mathbf{h})\mathbf{r}) \right) \mathbf{E}_{02} \end{aligned}$$

We obtained the inhomogeneous wave equation. According to the perturbation theory, it is necessary to find its particular solution. Since the continuum is uniform with an accuracy of the reciprocal lattice vector  $\mathbf{h}$ , the desired wave field is

delocalized. It means that the particular solution of Eq. (12) must have the form of a plane wave. The particular solution of the equation

$$\text{rot rot } \mathbf{E}_0 - \kappa_0^2 \mathbf{E}_0 = \mathbf{A} \exp(i\mathbf{q}\mathbf{r})$$

takes the form

$$\mathbf{E} = \frac{\mathbf{A} \exp(i\mathbf{q}\mathbf{r})}{q^2 - \kappa_0^2} \quad (13)$$

Eq. (13) is obtained taking into account the condition  $\text{div } \mathbf{D} = 0$  from which follows  $(\boldsymbol{\kappa}_0 \mathbf{E}_{0i}) = (h \mathbf{E}_{0i}) = 0$   $i = 1, 2$ , that is, the field is strictly transverse when sources are absent.

Now, the solution in the first order of the perturbation theory can be written:

$$\begin{aligned} \mathbf{E}_1 = & \kappa^2 \frac{\mathbf{E}_{01} \exp(i(\boldsymbol{\kappa}_0 + \mathbf{h})\mathbf{r})}{(\boldsymbol{\kappa}_0 + \mathbf{h})^2 - \kappa_0^2} + \kappa^2 \frac{\chi_{\bar{H}}}{\chi_H} \frac{\mathbf{E}_{01} \exp(i(\boldsymbol{\kappa}_0 - \mathbf{h})\mathbf{r})}{(\boldsymbol{\kappa}_0 - \mathbf{h})^2 - \kappa_0^2} \\ & + \kappa^2 \frac{\mathbf{E}_{02} \exp(-i(\boldsymbol{\kappa}_0 - \mathbf{h})\mathbf{r})}{(\boldsymbol{\kappa}_0 - \mathbf{h})^2 - \kappa_0^2} + \kappa^2 \frac{\chi_{\bar{H}}}{\chi_H} \frac{\mathbf{E}_{02} \exp(-i(\boldsymbol{\kappa}_0 + \mathbf{h})\mathbf{r})}{(\boldsymbol{\kappa}_0 + \mathbf{h})^2 - \kappa_0^2} \end{aligned} \quad (14)$$

Finally, the direct expansion with an accuracy of  $\chi_H^2$  takes the form

$$\begin{aligned} \mathbf{E}(\mathbf{r}) = & \mathbf{E}_0(\mathbf{r}) + \chi_H \mathbf{E}_1(\mathbf{r}) + \dots = \\ = & \mathbf{E}_{01} \left( \exp(i\boldsymbol{\kappa}_0 \mathbf{r}) + \kappa^2 \chi_H \frac{\exp(i(\boldsymbol{\kappa}_0 + \mathbf{h})\mathbf{r})}{(\boldsymbol{\kappa}_0 + \mathbf{h})^2 - \kappa_0^2} + \kappa^2 \chi_{\bar{H}} \frac{\exp(i(\boldsymbol{\kappa}_0 - \mathbf{h})\mathbf{r})}{(\boldsymbol{\kappa}_0 - \mathbf{h})^2 - \kappa_0^2} \right) + \\ & \mathbf{E}_{02} \left( \exp(-i\boldsymbol{\kappa}_0 \mathbf{r}) + \kappa^2 \chi_H \frac{\exp(-i(\boldsymbol{\kappa}_0 - \mathbf{h})\mathbf{r})}{(\boldsymbol{\kappa}_0 - \mathbf{h})^2 - \kappa_0^2} + \kappa^2 \chi_{\bar{H}} \frac{\exp(-i(\boldsymbol{\kappa}_0 + \mathbf{h})\mathbf{r})}{(\boldsymbol{\kappa}_0 + \mathbf{h})^2 - \kappa_0^2} \right) + \dots \end{aligned} \quad (15)$$

It follows from Eq. (15) that in addition to the direct ( $\boldsymbol{\kappa}_0$ ) and inverse ( $-\boldsymbol{\kappa}_0$ ) directions of the plane wave propagation in a continuum, waves in the directions  $(\boldsymbol{\kappa}_0 \pm \mathbf{h})$  and  $-(\boldsymbol{\kappa}_0 \pm \mathbf{h})$  appear as well. The amplitude of these waves is negligibly small ( $\chi_H$  times smaller) as compared to the initial one and cannot substantially change the wave field in the crystal. Thus, the refracted (and also possibly reflected) wave with small distortions propagates in the crystal.

However, this position radically changes when any denominator in Eq. (15) approaches zero. In this case  $\mathbf{E}_1 \rightarrow \infty$ , and we cannot consider a small correction to  $\mathbf{E}_0$ . Then, the direct expansion does not hold, and its modification is required. Apparently, this occurs under condition

$$(\boldsymbol{\kappa}_0 \pm \mathbf{h})^2 - \kappa_0^2 \leq \chi_H$$

This condition is well known: it is the Laue condition for X-rays, and therefore there is no need to detail its physical sense. Note only that all geometric constructions following from the Laue condition appear in this case as a natural consequence of validity violation of the direct field expansion in the parameter  $\chi_H$ .

Thus, the wave field structure principally changes for certain  $\boldsymbol{\kappa}_0$  values, and new directions of the wave propagation different from the initial one appear, that is, diffraction. We will restrict ourselves here and below to the two-wave approximation when the transmitted and diffracted waves satisfy the Laue equation.

Thus, it is necessary to modify the direct expansion near the  $\boldsymbol{\kappa}_0$  values for which diffraction is observed. The parametric character of the interaction of continuum

with a wave field is the principal moment here which provides the physical (and mathematical) justification for the search of the solution.

There are different methods to modify the direct expansion. All of them are directed to solve one problem: to obtain a so-called uniformly acceptable expansion near the values of parameters interesting for us. The method of multiple scales is most favorable for our investigation [9]. However, method modification is necessary having in mind the vector character of the problem.

### 2.3 The method of multiple scales

The main idea of the method for the considered problem is the following. The wave field singularities appear for different spatial scales determined by a small parameter of expansion of  $\chi_H$ . Correspondingly, these singularities can be independently considered in the specified approximation. It is attained mathematically by the transition from one spatially variable ( $\mathbf{r}$  in our case) to several ones reflecting different scales of the problems. The fixed number of scales determines the expansion order of the solution. The abovementioned modification is related to the fact that the method of many scales is used for scalar equations; here, it is used for the vector equation.

Thus, we will search for the approximate solution of Eq. (10) for the most interesting case in the area of the Bragg maximum when the Laue condition  $\mathbf{\kappa}_0 \pm \mathbf{h} = \mathbf{\kappa}_h$  is fulfilled. We make the substitution  $\mathbf{r} \rightarrow \mathbf{r}_0, \mathbf{r}_{1,\dots} = \mathbf{r}_0, \chi_H \mathbf{r}_0, \dots$  in Eq. (10), assuming that the field is determined by different spatial scales:

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}(\mathbf{r}_0, \mathbf{r}_1, \dots).$$

Hereinafter, we will restrict ourselves to the first order of expansion; correspondingly, we will consider two spatial scales  $\mathbf{r}_0$  and  $\mathbf{r}_1$ .

Then, for  $\text{rot}\mathbf{E}$  we obtain

$$\text{rot}\mathbf{E} = (\text{rot}_0 + \chi_H \text{rot}_1 + \dots)\mathbf{E}$$

that is, operator  $\text{rot}$  is linear relative to the carried-out substitution. The index of the operator signifies the space in which it operates. Using this property we obtain

$$\begin{aligned} \text{rotrot} &= (\text{rot}_0 + \chi_H \text{rot}_1 + \dots)(\text{rot}_0 + \chi_H \text{rot}_1 + \dots) = \\ &= \text{rot}_0 \text{rot}_0 + \chi_H \text{rot}_1 \text{rot}_0 + \chi_H \text{rot}_0 \text{rot}_1 + \dots \end{aligned}$$

As was indicated above, the interaction of the field with continuum has a parametric character. This means that along with the field expansion it is also necessary to expand the wave vector  $\mathbf{\kappa}_0$  in powers of  $\chi_H$ :

$$\begin{aligned} \mathbf{E} &= \mathbf{E}_0(\mathbf{r}_0, \mathbf{r}_1, \dots) + \chi_H \mathbf{E}_1(\mathbf{r}_0, \mathbf{r}_1, \dots) + \dots; \\ \mathbf{\kappa}_0 &= \mathbf{\kappa}_{00} + \chi_H \mathbf{\kappa}_{01} + \dots; \end{aligned} \tag{16}$$

$$\kappa_0^2 = (\mathbf{\kappa}_0, \mathbf{\kappa}_0) = \kappa_0^2 + 2\chi_H (\mathbf{\kappa}_0, \mathbf{\kappa}_{01}) + \dots = \kappa_0^2 + \chi_H X; \quad X = 2(\mathbf{\kappa}_0, \mathbf{\kappa}_{01})$$

We substitute all expansions into Eq. (10):

$$\begin{aligned} &(\text{rot}_0 \text{rot}_0 + \chi_H \text{rot}_1 \text{rot}_0 + \chi_H \text{rot}_0 \text{rot}_1 + \dots)(\mathbf{E}_0 + \chi_H \mathbf{E}_1 + \dots) - \\ &- \left( \kappa_0^2 + \chi_H X + \dots + \kappa^2 \chi_H \left( \exp(i\mathbf{h}\mathbf{r}_0) + \frac{\chi_H}{\chi_H} \exp(-i\mathbf{h}\mathbf{r}_0) \right) \right) (\mathbf{E}_0 + \chi_H \mathbf{E}_1 + \dots) = 0 \end{aligned} \tag{17}$$



In this case,  $\chi(\mathbf{r})$  is presented as a function of the ground spatial scale  $\mathbf{r}_0$ . The subsequent procedure follows the standard scheme of perturbation methods.

Namely, the initial approximation (unperturbed state) and subsequent ones are obtained when the constants of powers of the perturbation parameter  $\chi_H$  are sequentially equated. The uniformly available expansion is obtained when additional conditions are imposed elimination of secular (divergent) terms of expansion. In turn, this elimination is due to the expansion of  $\kappa_0$  and introduction of different scales of the problem.

Let us demonstrate this procedure. As before the zeroth approximation, (the unperturbed equation) has the form of the standard vector wave equation for transverse waves propagating in continuum:

$$\text{rot}_0 \text{rot}_0 \mathbf{E}_0 - \kappa_{00}^2 \mathbf{E}_0 = 0. \quad (18)$$

However, in contrast to the direct expansion, the operator  $\text{rot}$  acts here only on the single spatial scale  $\mathbf{r}_0$ . According to this, the solution should search in the form of superposition of transmitted and diffracted waves (two-wave approximation):

$$\begin{aligned} \mathbf{E}_0 &= \mathbf{e}_1 c_1(\mathbf{r}_1) \exp(i\kappa_{00} \mathbf{r}_0) + \mathbf{e}_2 c_2(\mathbf{r}_1) \exp(i\kappa_h \mathbf{r}_0) \\ (\kappa_{00}, \mathbf{e}_i) &= (\kappa_h, \mathbf{e}_i) = 0. \end{aligned} \quad (19)$$

The quantities  $c_i(\mathbf{r}_1)$  are related to the other spatial scale and considered as slow variables.

This structure of the wave field supposes strict fulfillment of the diffraction Laue condition  $\kappa_0 \pm \mathbf{h} = \kappa_h$  and the presence of reflecting plane. In fact the condition  $(\kappa_0 \mathbf{h}) = \pm 1/2$  follows from  $(\kappa_0 \pm \mathbf{h})^2 - \kappa_0^2 = 0$  which imposes the limitation only on the component  $\kappa_0$  directed along  $\mathbf{h}$ ,  $\kappa_{0\parallel}$ . The component  $\kappa_{0\perp}$  normal to  $\mathbf{h}$  is identical for  $\kappa_0$  and  $\kappa_h$ .

The condition of wave transversity  $(\kappa_{00}, \mathbf{e}_i) = (\kappa_h, \mathbf{e}_i) = 0$  defines only the planes orthogonal to the corresponding wave vectors. As is known two cases of polarization are considered, namely,  $\sigma$  polarization when the field amplitude is in the plane orthogonal to the diffraction plane and  $\pi$  polarization when the field amplitude is in the diffraction plane. The case of  $\sigma$  polarization is more favorable for the further consideration being a simpler one.

The following first-order approximation to leads to the inhomogeneous equation:

$$\begin{aligned} \text{rot}_0 \text{rot}_0 \mathbf{E}_1 - \kappa_{00}^2 \mathbf{E}_1 &= -(\text{rot}_1 \text{rot}_0 + \text{rot}_0 \text{rot}_1) \mathbf{E}_0 + X \mathbf{E}_0 \\ &+ \kappa^2 (\exp(i\mathbf{h} \mathbf{r}_0) + \chi_{\bar{H}}/\chi_H \exp(-i\mathbf{h} \mathbf{r}_0)) \mathbf{E}_0 \end{aligned} \quad (20)$$

Hence

$$\begin{aligned} \text{rot}_0 \text{rot}_0 \mathbf{E}_1 - \kappa_{00}^2 \mathbf{E}_1 &= \left( (i2(\nabla_1 c_1, \kappa_{00}) + X c_1) \mathbf{e}_1 + \kappa^2 \frac{\chi_{\bar{H}}}{\chi_H} c_2 \mathbf{e}_2 \right) \exp(i\kappa_{00} \mathbf{r}_0) + \\ &+ (\kappa^2 c_1 \mathbf{e}_1 + (i2(\nabla_1 c_2, \kappa_h) + X c_2) \mathbf{e}_2) \exp(i\kappa_h \mathbf{r}_0) + \\ &+ \kappa^2 \frac{\chi_{\bar{H}}}{\chi_H} \exp(i(\kappa_{00} - \mathbf{h}) \mathbf{r}_0) c_1 \mathbf{e}_1 + \kappa^2 \exp(i(\kappa_h + \mathbf{h}) \mathbf{r}_0) c_2 \mathbf{e}_2. \end{aligned} \quad (21)$$

Operator  $\nabla_1$  (gradient) acts here on  $\mathbf{r}_1$ . Eq. (21) is obtained taking into account  $(\kappa_{00} \mathbf{e}) = (\kappa_h \mathbf{e}) = 0$  and the additional condition  $(\nabla_1 c_1, \mathbf{e}_1) = 0$ . This means the following. The quantities  $c_i(\mathbf{r}_1)$  are considered as the perturbed amplitudes of the corresponding plane waves. The two first terms in the right side of Eq. (21) generate the secular components in expansion which is seen from the abovementioned

particular solution. In other words they provide parametric resonance in the system. Consequently, it is necessary to eliminate these terms in order to obtain the uniform approximation near the Laue condition. Then, we obtain the following system of vector equations:

$$\begin{cases} (i2(\nabla_1 c_1, \mathbf{\kappa}_{00}) + Xc_1)\mathbf{e}_1 + \kappa^2 \frac{\chi_H}{\chi_H} c_2 \mathbf{e}_2 = 0 \\ (i2(\nabla_1 c_2, \mathbf{\kappa}_h) + Xc_2)\mathbf{e}_2 + \kappa^2 c_1 \mathbf{e}_1 = 0 \end{cases} \quad (22)$$

In contrast to the usual scalar system, additional limitations are necessary to solve Eq. (22). The issue is that  $\mathbf{e}_1$  and  $\mathbf{e}_2$  are linearly independent in a general case (e.g., for  $\pi$  polarization), that is, form a certain vector basis. It is clear that in the general case it is not possible to provide the field limitations in all the space if one has only the given system. Therefore, it is necessary to select the characteristic directions (or planes orthogonal to them) along which the field limitation is realized, that is, the obtained solution proves to be uniformly available. According to the physical meaning of the problem, one can assume that these directions are related to the transmitted ( $\mathbf{\kappa}_{00}$ ) and diffracted ( $\mathbf{\kappa}_h$ ) waves. This assumption is confirmed by the following.

The particular solution of the inhomogeneous equation

$$\text{rotrot}\mathbf{E} - \kappa_0^2 \mathbf{E} = \mathbf{e} \exp(i\mathbf{\kappa}_0 \mathbf{r})$$

in the resonance case takes the form

$$\mathbf{E} = \left( \frac{i(\mathbf{\kappa}_0 \mathbf{r})}{2\kappa^2} \mathbf{e} - \frac{(\mathbf{\kappa}_0 \mathbf{e})}{\kappa^4} \mathbf{\kappa}_0 - \frac{i(\mathbf{\kappa}_0 \mathbf{e})(\mathbf{\kappa}_0 \mathbf{r})}{2\kappa^4} \mathbf{\kappa}_0 \right) \exp(i\mathbf{\kappa}_0 \mathbf{r}).$$

It is seen from here that the infinite increase in the wave amplitude is associated with the wave vector  $\mathbf{\kappa}_0$  in the direction coinciding with  $\mathbf{e}$ . Then, according to the meaning of the zeroth approximation, it is necessary that the projections onto  $\mathbf{e}_1$  in the first equation of Eq. (22) vanish and analogously the projections onto  $\mathbf{e}_2$  in the second equation vanish.

Thus, multiplying scalarly the first equation of the system by  $\mathbf{e}_1$  and the second one by  $\mathbf{e}_2$ , we obtain the scalar system

$$\begin{cases} i2(\nabla_1 c_1, \mathbf{\kappa}_{00}) + Xc_1 + \kappa^2 \frac{\chi_H}{\chi_H} \eta c_2 = 0 \\ \kappa^2 \eta c_1 + i2(\nabla_1 c_2, \mathbf{\kappa}_h) + Xc_2 = 0 \end{cases} \quad (23)$$

where

$$\eta = (\mathbf{e}_1 \mathbf{e}_2) = \begin{cases} 1 - \text{for } \sigma \text{ polarization} \\ \cos 2\theta - \text{for } \pi \text{ polarization} \end{cases}$$

The obtained system (23) is virtually the dispersion relation written in the differential form for the transmitted and diffracted waves in the two-wave approximation. As follows from the presented conclusion, the possibility to obtain this system is dictated by the choice of the zeroth approximation. Namely, the wave vectors of transmitted and diffracted waves must have the identical component  $\kappa_{0\perp}$  that leads to the scattering interpretation as a result of reflection from the atomic plane.

We pass from the differential form of system (23) to the algebraic one; for this purpose we make the following substitution  $c_j(\mathbf{r}_1) \rightarrow c_j \exp(i\mathbf{P}\mathbf{r})$ ,  $\nabla_1 c_j = i\mathbf{P}c_j$ , where  $\mathbf{P}$  is a certain constant vector.

We obtain

$$\begin{cases} (-2(\mathbf{P}\boldsymbol{\kappa}_{00}) + X)c_1 + \kappa^2 \frac{\chi_{\bar{H}}}{\chi_H} \eta c_2 = 0 \\ \kappa^2 \eta c_1 + (-2(\mathbf{P}\boldsymbol{\kappa}_h) + X)c_2 = 0 \end{cases} \quad (24)$$

This system should be considered as the condition of field limitation in the specified direction of field propagation that is related to the structure parameters of the crystal and to the diffraction geometry. As for the physical meaning of the considered problem, this limitation should be in the direction of the normal inside crystal.

$$\begin{cases} (-2P\kappa_{00}\gamma_0 + X)c_1 + \kappa^2 \eta \frac{\chi_{\bar{H}}}{\chi_H} c_2 = 0 \\ \kappa^2 \eta c_1 + (-2P\kappa_h\gamma_h + X)c_2 = 0 \end{cases} \quad (25)$$

Here,  $\gamma_{0,h}$  are the direction cosines of the corresponding wave vectors,  $\kappa_h = \kappa_{00}$ . The nontrivial solution of Eq. (25) requires the corresponding determinant to vanish:

$$4\kappa_{00}^2 \gamma_n \gamma_0 P^2 - 2\kappa_{00} X (\gamma_0 + \gamma_h) P + X^2 - \kappa^4 \eta^2 \frac{\chi_{\bar{H}}}{\chi_H} = 0 \quad (26)$$

The solution of quadratic equation relative to  $P$  takes the form

$$P_{1,2} = \frac{X(\gamma_0 + \gamma_h) \pm \left[ X^2(\gamma_0 - \gamma_h)^2 + 4\gamma_0\gamma_h\kappa^4\eta^2 \frac{\chi_{\bar{H}}}{\chi_H} \right]^{1/2}}{4\kappa_{00}\gamma_h\gamma_0} = \frac{X(\gamma_0 + \gamma_h) \pm D}{4\kappa_{00}\gamma_h\gamma_0} \quad (27)$$

Then, solving, for example, the first equation of system (25) relative to  $c_2$ , we obtain

$$c_2 = \frac{X(\gamma_0 - \gamma_h) \pm D}{2\kappa^2 \eta \gamma_h} \cdot \frac{\chi_H}{\chi_{\bar{H}}} c_1 = \alpha_{1,2} c_1 \quad (28)$$

Finally, going back to the initial variables, we represent the wave field in the crystal in the following form:

$$\begin{aligned} \mathbf{E} = & \exp(i\chi_H(\mathbf{P}_1\mathbf{r})) (\exp(i\boldsymbol{\kappa}_{00}\mathbf{r})\mathbf{e}_1 + \alpha_1 \exp(i\boldsymbol{\kappa}_h\mathbf{r})\mathbf{e}_2) c_{11} \\ & + \exp(i\chi_H(\mathbf{P}_2\mathbf{r})) (\exp(i\boldsymbol{\kappa}_{00}\mathbf{r})\mathbf{e}_1 + \alpha_2 \exp(i\boldsymbol{\kappa}_h\mathbf{r})\mathbf{e}_2) c_{12} \end{aligned} \quad (29)$$

Here, the constants  $c_{ij}$  have the additional indices corresponding to the values of  $P_1$  and  $P_2$ .

The equation for the wave field is simplified for the case of semi-infinite crystal when the wave reflection from a lower crystal face is eliminated. In this case the choice of sign in  $P_{1,2}$  and correspondingly in  $\alpha_{1,2}$  is defined by physical considerations. Namely, it is necessary that the wave field transfers to the usual form of the refracted wave propagating in the crystal as continuum at the deviation from the exact Bragg condition (increasing  $|X|$ ). Then, we have

$$P = \frac{X(\gamma_0 + \gamma_h) - \text{sgn}(X)D}{4\kappa_{00}\gamma_h\gamma_0}; \quad (30)$$

$$\alpha = \frac{X(\gamma_0 - \gamma_h) - \text{sgn}(X)D}{2\kappa^2 \eta \gamma_h \chi_{\bar{H}} / \chi_H} \quad (31)$$

$$\text{sgn}(X) = \begin{cases} 1, & X \geq 0 \\ -1, & X < 0 \end{cases}$$

Finally, the wave field in the crystal takes the form

$$\mathbf{E} = \exp(i\chi_H(\mathbf{Pr}))(\exp(i\boldsymbol{\kappa}_{00}\mathbf{r})\mathbf{e}_1 + \alpha \exp(i\boldsymbol{\kappa}_h\mathbf{r})\mathbf{e}_2)c \quad (32)$$

where the constant  $c$  is determined from the boundary conditions.

Eq. (32) describes the uniform wave field in a perfect crystal near the Bragg maximum.

To compare the obtained expression to the known results and to the experiment, it is necessary to go to the angular variable which connects with the deviation from the exact Bragg angle  $\Delta\theta$ . In this case, the parameter  $X = 2(\boldsymbol{\kappa}_{00}\boldsymbol{\kappa}_{01})$  should be expressed by  $\Delta\theta$ . As was mentioned the parametric resonance (diffraction Laue condition  $(\boldsymbol{\kappa}_0\mathbf{h}) = \mp 1/2$ ) is determined only by the component  $\boldsymbol{\kappa}_{0\parallel}$  directed along  $\mathbf{h}$ , by the vector character of the problem. This means that the vector  $\boldsymbol{\kappa}_{01}$  in expansion  $\boldsymbol{\kappa}_0 = \boldsymbol{\kappa}_{00} + \chi_H\boldsymbol{\kappa}_{01}$  is directed along  $\mathbf{h}$ ,  $\boldsymbol{\kappa}_{01} = \kappa_{01}\mathbf{h}$ . Taking into account that the reflection fixed in the experiment is determined by the normal component of the wave vector  $\kappa_{0n} = (\boldsymbol{\kappa}_0\mathbf{n})$ , we obtain for  $X$

$$X = -\frac{\kappa_{00}^2\beta_H\gamma_0}{(\gamma_h - \gamma_0)\chi_H} \quad (33)$$

Here, we introduce the standard (with an accuracy of refraction) angular variable:

$$\beta_H = -2\Delta\theta \sin 2\theta$$

As is known, two principal schemes are considered in the diffraction theory, by Laue ( $\gamma_0 > 0, \gamma_h > 0$ ) and by Bragg ( $\gamma_0 > 0, \gamma_h < 0$ ). In the case of Bragg diffraction, the wave field structure will qualitatively differ depending on the considered angular range.

In particular in the range

$$X^2(\gamma_0 + |\gamma_h|)^2 < 4\gamma_0|\gamma_h|\kappa^4\eta^2\frac{\chi_H}{\chi_H},$$

the waves will exponentially attenuate along the normal surface into the crystal. In terms of the qualitative theory of differential equations, the solution will be unstable. The known interpretation [10, 11] leads to the conclusion of the expulsion of the wave from the crystal and the formation of a diffraction maximum. Thus, the indicated condition separates the stable solutions (oscillating type) from unstable ones (exponential type), that is, provides the equations of transition curves of the parametric plane  $(X, \kappa^2)$  [10, 11].

The width of the unstable region, the region of exponential wave attenuation, is determined by the expression

$$\Delta X = \frac{4\kappa^2\eta(\gamma_0|\gamma_h|)^{1/2}}{\gamma_0 + |\gamma_h|} \cdot \left(\frac{\chi_H}{\chi_H}\right)^{1/2} \quad (34)$$

or proceeding to the angular variable

$$\Delta\theta = \frac{2\eta(\chi_H\chi_H)^{1/2}}{(1 + \chi_0) \sin 2\theta} \cdot \left(\frac{|\gamma_h|}{\gamma_0}\right)^{1/2} \quad (35)$$

This is the known expression (with an accuracy of refraction) for the angular width of the Bragg table for the case of the semi-infinite perfect non-absorbing crystal. The extinction length  $\Lambda_{ext}$  is determined as a decrement of wave attenuation in the point Bragg position:

$$\Lambda_{ext} = \frac{2\kappa_{00}(|\gamma_h|\gamma_0)^{1/2}}{\kappa^2\eta(\chi_{\bar{H}}\chi_H)^{1/2}} \approx \frac{\kappa}{|\chi_H|} \quad (36)$$

We now summarize the intermediate stage. The use of the generalized method of many scales allowed us to obtain the system of basic equations describing the behavior of wave field near the Bragg maximum in the two-wave approximation. This system is a direct analog of the dispersion relations of the Ewald-Laue theory and the Takagi-Taupin system of the generalized dynamic theory. The substantial difference of the developed variant of the theory consists in the cancelation of the shortening procedure of equations by neglecting the second derivatives. The principal moment here is the expansion in  $\chi_H$  which makes it possible to save maximally the structure of Maxwell equations for the wave field in the crystal under conditions of the dynamic diffraction.

Comparison of the obtained results to that known from the Takagi-Taupin theory shows the complete correspondence both in the qualitative interpretation of types of the solutions obtained in the different angular ranges in the case of Bragg diffraction and in the analytical expressions for the width of the Bragg maximum and the extinction length. This correspondence indicates that in spite of the formal representation of  $\chi(\mathbf{r})$  in the form of infinite Fourier series in the Ewald-Laue and Takagi-Taupin theories only three terms of the series are really used.

However, the value of the theory developed here shows itself to a large degree when the boundary conditions are taken into account that takes the explicit expressions for the reflection coefficient. Therefore, we consider now the boundary conditions and determine the principal difference between our approach and known variants of the dynamical diffraction theory.

## 2.4 Boundary conditions and the amplitude reflection coefficient

According to Eq. (32), the expression above obtained for the wave field in the crystal depends on the constant  $c$ , which must be determined by the boundary conditions of the problem. As was indicated above, it is not possible to use the classical boundary conditions of electrodynamics in the Takagi-Taupin theory since negligibility of the second derivatives of amplitudes with respect to the coordinates reduces the order of the equation. As a result the boundary conditions redefine the problem, and the new boundary conditions are stated that determine only the field amplitudes on a crystal surface. This procedure proves to be quite correct for usual diffraction geometries, when the angles of incidence and yield of waves substantially exceed the critical values.

We find out now the differences appearing when the boundary conditions are strictly taken into account in our theory.

The reflection coefficient is determined as a ratio of the averaged values of normal components of the pointing vector for the diffracted and incident waves:

$$R = \left| \frac{c_h^0}{c^0} \right|^2 \cdot \frac{(\mathbf{n}\boldsymbol{\kappa}_h^0)}{(\mathbf{n}\boldsymbol{\kappa})} \quad (37)$$

Here,  $\mathbf{n}$  is the unit vector of the normal directed inside the crystal, and  $\boldsymbol{\kappa}$ ,  $c^0$  and  $\boldsymbol{\kappa}_h^0$ ,  $c_h^0$  are the wave vectors and amplitudes of the incident and diffracted waves,



respectively. Index 0 denotes that the values of the indicated quantities are related to the environment vacuum. Thus, the determination of the reflection coefficient is associated with the determination of the diffracted wave amplitude in the vacuum. This problem is solved by the boundary conditions.

As is known, the boundary conditions require continuity of the tangential components of electric and magnetic fields which is a consequence of the uniformity of the problem along the surface. The boundary problem disintegrates into successive steps related to the determination of  $c_h^0$ . In this case the elementary problem is considered at each stage, namely, the determination of the relation between the amplitudes of incident, transmitted, and secularly reflected waves. The solution of this problem leads to the known Fresnel formulas:

$$c = \frac{(\mathbf{n}, \boldsymbol{\kappa}) - (\mathbf{n}, \boldsymbol{\kappa}_R)}{(\mathbf{n}, \boldsymbol{\kappa}_0 + \mathbf{P}) - (\mathbf{n}, \boldsymbol{\kappa}_R)} c^0 = \frac{2(\mathbf{n}, \boldsymbol{\kappa})}{(\mathbf{n}, \boldsymbol{\kappa}_0 + \mathbf{P}) + (\mathbf{n}, \boldsymbol{\kappa})} c^0 \quad (38)$$

$$c_R = \frac{(\mathbf{n}\boldsymbol{\kappa}) - (\mathbf{n}, \boldsymbol{\kappa}_0 + \chi_H \mathbf{P})}{(\mathbf{n}, \boldsymbol{\kappa}_0 + \chi_H \mathbf{P}) - (\mathbf{n}\boldsymbol{\kappa}_R)} c^0 = \frac{(\mathbf{n}\boldsymbol{\kappa}) - (\mathbf{n}, \boldsymbol{\kappa}_0 + \chi_H \mathbf{P})}{(\mathbf{n}, \boldsymbol{\kappa}_0 + \chi_H \mathbf{P}) + (\mathbf{n}\boldsymbol{\kappa})} c^0 \quad (39)$$

$$c_h^0 = \frac{(\mathbf{n}, \boldsymbol{\kappa}_h + \chi_H \mathbf{P}) - (\mathbf{n}, \boldsymbol{\kappa}_{hR})}{(\mathbf{n}, \boldsymbol{\kappa}_h^0) - (\mathbf{n}, \boldsymbol{\kappa}_{hR})} \alpha c = \frac{(\mathbf{n}, \boldsymbol{\kappa}_h + \chi_H \mathbf{P}) - (\mathbf{n}, \boldsymbol{\kappa}_{hR})}{(\mathbf{n}, \boldsymbol{\kappa}_h^0) - (\mathbf{n}, \boldsymbol{\kappa}_{hR})} \cdot \frac{2(\mathbf{n}, \boldsymbol{\kappa})}{(\mathbf{n}, \boldsymbol{\kappa}_0 + \chi_H \mathbf{P}) + (\mathbf{n}, \boldsymbol{\kappa})} \alpha c^0 \quad (40)$$

Here,  $c_R$  is the amplitude of the specularly reflected wave, and  $\boldsymbol{\kappa}_{hR}$  is the wave vector of the diffraction wave specularly reflected from the lower side of the crystal-vacuum interface.

The obtained relations allow us to determine not only the diffracted wave but also the specularly reflected wave, which principally distinguishes our approach from the formalism of the Takagi-Taupin equations.

Eqs. (38)–(40) solve the problem of the determination of field amplitudes under the conditions of sliding noncoplanar diffraction when the incident and diffracted waves are near the critical angles of total external reflection (TER). They are analogous to the relations obtained in [12] where this problem was solved by the fourth-order dispersion equation.

The correspondence with the Takagi-Taupin theory must be undoubtedly fulfilled for the case of large angles of incidence and yield of the diffraction wave. Really in this case, the amplitude of specular wave tends to be zero, and the reflection coefficient takes the form

$$R = \left| \frac{c_h^0}{c^0} \right|^2 \cdot \frac{(\mathbf{n}\boldsymbol{\kappa}_h^0)}{(\mathbf{n}\boldsymbol{\kappa})} = |\alpha|^2 \frac{(\mathbf{n}\boldsymbol{\kappa}_h^0)}{(\mathbf{n}\boldsymbol{\kappa})} \quad (41)$$

$$= \frac{\gamma_0(1 + \chi_0)\beta_H - \operatorname{sgn}(\beta_H) \left[ (\gamma_0(1 + \chi_0)\beta_H)^2 + 4\gamma_0\gamma_H\eta^2\chi_{\bar{H}}\chi_H \right]^{1/2}}{2\gamma_H\eta\chi_H} \cdot \frac{\gamma_H}{\gamma_0}$$

This is the known expression for the coefficient of reflection from a perfect half-infinite crystal, i.e. the Bragg table. In addition to this in the case of extremely asymmetric diffraction when the diffraction wave leaving the crystal is almost parallel to the surface, the amplitude is modulated by the factors taking into account the refraction of transmitted and diffracted waves at the crystal-vacuum interface and the diffraction wave interaction related to the vector  $\mathbf{P}$ .

The proposed covariant (it may be named nonstandard) theory allows the generalization for the case of the crystal with lattice deformations. Therefore, a

uniform approach to the account of deformations and other distortions in all diffraction schemes is realized.

### 3. Generalization of a covariant dynamic diffraction theory to the case of deformed crystal

It is known that Takagi-Taupin equations were obtained using the model concept of the character of lattice distortions which makes it possible to directly take into account the displacement of atomic planes in the three-dimensional periodic function of crystal polarizability. This concept allows for describing lattice displacements and strain using the methods of classical theory of elasticity formulated within the continuum approximation. To satisfy the condition of the dynamic character of scattering in the Takagi-Taupin theory, the lattice distortion is assumed to be rather weak; correspondingly, the strain is small. The character of variation in strain is implicitly taken into account only when the wave field is chosen in the form of a Bloch function with slowly varying amplitudes; thus, the question of applicability of this concept remains open.

There is another limitation of the Takagi-Taupin theory which is related to the correct statement of boundary conditions. Mathematically, the Takagi-Taupin equations form a first-order differential system with respect to the scalar amplitudes of transmitted and diffracted waves. The procedure of determining these amplitudes at the crystal-vacuum interface does not correspond to the classical boundary conditions.

This discrepancy is due to the fact that the Takagi-Taupin equations are obtained disregarding the second derivatives of the field amplitudes with respect to coordinates. Thus, the boundary conditions impose fundamental limitations on the applicability of the Takagi-Taupin equations (e.g., when analyzing extremely asymmetric diffraction schemes).

In this section we generalized the covariant theory of dynamic diffraction which was presented in the previous section, to a crystal with a distorted lattice. This approach makes it possible to formulate the limitation on the character of variation in strain for the applicability of the Takagi-Taupin equations. In addition, the equations obtained can be applied (as in the case of an ideal crystal) for arbitrary diffraction schemes.

In this section, we follow the original papers [13, 14].

#### 3.1 Wave field in the absence of diffraction

The polarizability  $\chi(\mathbf{r}')$  of a crystal with a distorted lattice is a function of coordinates; however, in contrast with an ideal crystal, it depends not only on the reciprocal lattice vector  $\mathbf{H}$  but also on the vector of atomic plane displacement from equilibrium  $\mathbf{u}(\mathbf{r}')$ . According to the accepted assumptions of the generalized dynamic theory, we choose the crystal model  $\chi(\mathbf{r}')$  in the form

$$\chi(\mathbf{r}') = \chi_0 + \chi_H \exp(i\mathbf{H}(\mathbf{r}' + \mathbf{u}(\mathbf{r}'))) + \chi_{\bar{H}} \exp(-i\mathbf{H}(\mathbf{r}' + \mathbf{u}(\mathbf{r}'))) \quad (42)$$

It can be seen that the general structure of  $\chi(\mathbf{r}')$  corresponds to the case of an ideal crystal. Obviously, this situation is possible only when the displacement  $\mathbf{u}(\mathbf{r}')$  is small. Then, for Eq. (7) we arrive at

$$\text{rot rot } \mathbf{E}(\mathbf{r}') - k^2 (1 + \chi_0 + \chi_H \exp(i\mathbf{H}(\mathbf{r}' + \mathbf{u}(\mathbf{r}'))) + \chi_{\bar{H}} \exp(-i\mathbf{H}(\mathbf{r}' + \mathbf{u}(\mathbf{r}')))) \mathbf{E}(\mathbf{r}') = 0 \quad (43)$$

As in the case of an ideal crystal, Eq. (43) should be reduced to a dimensionless form. To this end we will use the length  $\mathbf{H}$  of the reciprocal lattice vector:

$$\text{rotrot}\mathbf{E}(\mathbf{r}) - \kappa^2(1 + \chi_0 + \chi_H \exp(i\mathbf{h}(\mathbf{r} + \mathbf{u}(\mathbf{r}))) + \chi_{\bar{H}} \exp(-i\mathbf{h}(\mathbf{r} + \mathbf{u}(\mathbf{r}))))\mathbf{E}(\mathbf{r}) = 0; \quad (44)$$

The approximate solution to Eq. (44) in the Takagi-Taupin theory is known to be sought after in the form of plane waves with slowly varying amplitudes. Finally, the Takagi-Taupin equations can be derived from Eq. (44) with allowance for the two-wave approximation [2].

The covariant dynamic theory in the case of an ideal crystal is due to the fact that the Fourier component of polarizability  $\chi_H$  which is responsible for the excitation of a diffraction wave in the crystal under the corresponding Laue geometric condition for the wave vectors of refracted and diffracted waves and the reciprocal lattice vector was chosen to be the perturbation parameter. The parameter  $\chi_0$  cannot be considered a perturbation parameter because it leads to only refraction of the incident wave in the crystal and does not influence the occurrence of diffraction effects. Obviously, in the case of a weakly deformed crystal, the criterion of the choice of  $\chi_H$  as the expansion parameter remains valid because the presence of a weak displacement field only transforms the diffraction pattern rather than breaking it. This circumstance allows one to extend (with necessary modifications) the scheme of constructing a solution in the nonstandard approach to a deformed structure.

Recall that in the case of an ideal crystal the direct expansion of the solution to Eq. (44) in the parameter  $\chi_H$  is inconsistent when a parametric resonance is observed which corresponds to the Laue diffraction condition:

$$(\kappa_0 \pm \mathbf{h})^2 - \kappa_0^2 = 0 \quad (45)$$

In this case, the scattered wave amplitude increases unlimitedly. This is due to the fact that the diffraction wave can be found as a particular solution to the inhomogeneous wave equation:

$$\text{rotrot}\mathbf{E} - \kappa_0^2\mathbf{E} = \mathbf{E}_0 \exp(i(\kappa_0 \pm \mathbf{h})\mathbf{r}) \quad (46)$$

which according to Eq. (13) has the form

$$\mathbf{E} = \frac{\mathbf{E}_0 \exp(i(\kappa_0 \pm \mathbf{h})\mathbf{r})}{(\kappa_0 \pm \mathbf{h})^2 - \kappa_0^2} \quad (47)$$

For a deformed crystal, the plane wave is replaced with  $\mathbf{E}_0 \exp(i(\mathbf{q}\mathbf{r} \pm \mathbf{h}\mathbf{u}(\mathbf{r})))$  within model (42); as a result a particular solution to Eq. (46) cannot be written in the form as in Eq. (47). A particular solution (Eq. (47)) can generally be represented in the integral form using Green's function for the corresponding homogeneous equation. However, the generality of this representation is devalued by the difficulties in analyzing the relations (e.g., in view of the vector character of the problem Green's function has generally speaking a tensor form). As a result the integral representation of the solution to Eq. (46) is basically formal.

At the same time from the physical point of view, the displacement field changes significantly at distances much larger than the lattice parameter. This limitation is substantiated in particular by the fact that we describe lattice distortions within the continuum approximation. In this case the approximate solution to Eq. (46) can be obtained similarly to Eq. (47):

$$\mathbf{E} = \frac{\mathbf{E}_0 \exp(i(\boldsymbol{\kappa}_0 \pm \mathbf{h})\mathbf{r} \pm i\mathbf{h}\mathbf{u}(\mathbf{r}))}{(\boldsymbol{\kappa}_0 \pm \mathbf{h})^2 - \kappa_0^2} \quad (48)$$

Correspondingly, the direct expansion of the solution to Eq. (44) for a deformed crystal is similar to that for an ideal crystal and is determined by the wave superposition in the form

$$\mathbf{E}_{01(2)} \left( \exp(i\boldsymbol{\kappa}_0\mathbf{r}) + \kappa^2 \chi_{H(\bar{H})} \frac{\exp(i(\boldsymbol{\kappa}_0 \pm \mathbf{h})\mathbf{r} \pm i\mathbf{h}\mathbf{u}(\mathbf{r}))}{(\boldsymbol{\kappa}_0 \pm \mathbf{h})^2 - \kappa_0^2} \right) \quad (49)$$

where  $\mathbf{E}_{01}$  and  $\mathbf{E}_{02}$  are the amplitudes of the plane waves  $\exp(\pm i\boldsymbol{\kappa}_0\mathbf{r})$  propagating in the crystal, considering a continuous medium with  $\chi = 1 + \chi_0$ . This solution describes the wave field in the crystal with a distorted lattice beyond the angular ranges of diffraction reflection (i.e., in the nonresonant case). The question of the accuracy of approximation (49) remains open until the character of the change in  $\mathbf{u}(\mathbf{r})$  is specified.

The most general limitation on the strain in the crystal is imposed by the requirement for the smallness of the strain tensor  $\boldsymbol{\varepsilon}$  corresponding to a given displacement field:

$$\boldsymbol{\varepsilon} = \varepsilon_0 \frac{\partial \mathbf{u}(\mathbf{r})}{\partial \mathbf{r}} \ll 1, \quad (50)$$

where  $\varepsilon_0$  is the strain amplitude in the structure. For sufficiently regular displacement fields, this requirement is reduced to the condition  $\varepsilon_0 \ll 1$ . It follows from Eq. (50) that in the case of a deformed crystal when the aforementioned conditions are satisfied the applicability of direct expansion remains limited because of the Laue resonant condition (45) where the amplitudes of waves excited in the crystal increase unlimitedly. Thus, the method for obtaining an approximate solution must also be modified in the case of a crystal with a distorted lattice. The choice of the modification technique depends on the character of the displacement field in the crystal and obviously cannot provide a universal solution for all physically possible cases. We will consider the most widespread situation where the displacement field changes at distances comparable with the extinction length. In this case the multiscale method which is the basis of the covariant theory of diffraction in an ideal crystal can directly be extended to a deformed structure.

### 3.2 Derivation of the main equations for strained crystal

The strain field in a crystal may have various forms depending on the nature of lattice distortions. These forms can mathematically be represented by setting different structural parameters (e.g., the thicknesses of epitaxial layers and transition regions between layers, sizes of lattice-strain regions caused by various defects, etc.). The values of these parameters are determined by not only the strain amplitudes  $\varepsilon_{0i}$  but also the characteristic regions  $L_i$  of their variation in the crystal. As a result this situation can symbolically be presented in a form that explicitly relates the parameters:

$$\mathbf{H}\mathbf{u} = F\left(\frac{\varepsilon_{0i}L_i}{d}, \frac{\mathbf{r}d}{L_i}\right) \quad (51)$$

Here,  $\varepsilon_0 L_i/d$  is the amplitude of the displacement field, and  $\mathbf{r}d/L_i$  is the size of the distorted region in the accepted coordinate normalization ( $d$  is the interplanar spacing). The influence of the factor  $\mathbf{Hu}$  on the diffraction effects should correlate with  $\chi_H$  which physically determines the characteristic region of wave-field formation under dynamic diffraction conditions. This concerns both the angular range of diffraction reflection and the field extinction length in the crystal.

Thus, the parameter  $\chi_H$  must implicitly be taken into account in functional relation (51) which takes the form

$$\mathbf{Hu} = F\left(\frac{\varepsilon_0}{m_i \chi_H^i}, m_i \mathbf{r}_i\right), m_i = \frac{1}{HL \chi_H^i} = \frac{d}{2\pi L \chi_H^i}, \mathbf{r}_i = \chi_H^i \mathbf{r}. \quad (52)$$

The powers  $i$  in Eq. (52) can be integers; however, fractional values (e.g., 1/2) are physically most interesting because they indicate changes in displacement fields on scales below the extinction length.

Thus, a consideration of different types of lattice distortions generally calls for taking into account different characteristic spatial regions; this approach completely corresponds to the main concept of the multiscale method [9]. Obviously, different modifications of the method are required depending on the specific structure of Eq. (52). We will consider the simplest case of one scale which leads in a particular case to Takagi-Taupin equations.

Let us consider the atomic plane displacement occurring at some effective layer thickness  $L$ . The parameter  $\mathbf{Hu}(\mathbf{r})$  can be written as

$$\mathbf{Hu}(\mathbf{r}) = \varepsilon_0 L H F\left(\frac{\mathbf{r}}{L}\right), \quad (53)$$

where  $F\left(\frac{\mathbf{r}}{L}\right)$  is the displacement model and  $\varepsilon_0$  is the strain amplitude.

According to the multiscale method [9], the main equation (Eq. (44)) is analyzed near the Bragg maximum on different spatial scales (determined by  $\chi_H$ ) using the transition from one variable  $\mathbf{r}$  to several variables  $\mathbf{r}_0 = \mathbf{r}$ ,  $\mathbf{r}_1 = \chi_H \mathbf{r}$ ,  $\mathbf{r}_2 = \chi_H^2 \mathbf{r}$ , ... If one seeks the first-order approximation for  $\chi_H$ , two scales (affecting the field in the crystal) should be considered:

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}(\mathbf{r}_0, \mathbf{r}_1).$$

Then, according to Section 2, the field, the operator  $\text{rot}$ , and the wave vector  $\mathbf{\kappa}_0$  are expanded in  $\chi_H$  powers:

$$\begin{aligned} \mathbf{E} &= \mathbf{E}_0(\mathbf{r}_0, \mathbf{r}_1) + \chi_H \mathbf{E}_1(\mathbf{r}_0, \mathbf{r}_1) + \dots; \\ \mathbf{\kappa}_0 &= \mathbf{\kappa}_{00} + \chi_H \mathbf{\kappa}_{01} + \dots; \end{aligned} \quad (54)$$

$$\kappa_0^2 = (\mathbf{\kappa}_0, \mathbf{\kappa}_0) = \kappa_0^2 + 2\chi_H (\mathbf{\kappa}_0, \mathbf{\kappa}_{01}) + \dots = \kappa_0^2 + \chi_H X; \quad X = 2(\mathbf{\kappa}_0, \mathbf{\kappa}_{01})$$

$$\text{rot rot} = \text{rot}_0 \text{rot}_0 + \chi_H (\text{rot}_0 \text{rot}_1 + \text{rot}_1 \text{rot}_0) + \dots$$

Substituting expansion (54) into the main equation (Eq. (44)), we obtain

$$\begin{aligned} &(\text{rot}_0 \text{rot}_0 + \chi_H \text{rot}_1 \text{rot}_0 + \chi_H \text{rot}_0 \text{rot}_1 + \dots)(\mathbf{E}_0 + \chi_H \mathbf{E}_1 + \dots) - \\ &-(\kappa_0^2 + \chi_H X + \dots + \kappa^2 \chi_H (\exp(i\mathbf{h}\mathbf{r}_0 + i\phi(\mathbf{r}_1)) + \\ &\frac{\chi_H}{\chi_H} \exp(-i\mathbf{h}\mathbf{r}_0 - i\phi(\mathbf{r}_1))))(\mathbf{E}_0 + \chi_H \mathbf{E}_1 + \dots) = 0 \end{aligned} \quad (55)$$



In contrast to the case of an ideal crystal,  $\chi(\mathbf{r})$  is now presented as a function of two spatial scales:  $\mathbf{r}_0$  and  $\mathbf{r}_1$ . Here, the following designation is introduced:

$$\phi(\mathbf{r}_1) = \frac{\varepsilon_0}{m\chi_H} \mathbf{H}\mathbf{u}(m\mathbf{r}_1), m = \frac{1}{HL\chi_H} = \frac{d}{2\pi L\chi_H}. \quad (56)$$

The parameter  $1/m$  means some effective thickness of the deformed layer on the scale  $\mathbf{r}_1$ . The possibility of presenting the displacement as a function of the scale  $\mathbf{r}_1$  suggests the condition  $m \sim 1$ , i.e., the number  $d$  of interplanar spacings embedded in the deformed layer thickness should be on the order of the extinction length  $\Lambda_{ext}$  on the dimensionless scale  $\mathbf{r}$ :

$$\frac{L}{d} \sim \frac{1}{\chi_H} \sim \Lambda_{ext} \quad (57)$$

We will follow the scheme for solving Eq. (55) that was reported in Section 1. As for an ideal crystal, the initial approximation can be written in the form as in Eq. (18). Accordingly, the operator  $\text{rot}$  acts on only one spatial scale  $\mathbf{r}_0$ . Since we are interested in the wave field near the Bragg maximum, a solution to Eq. (18) within the two-wave approximation should be sought after in the form of a superposition of transmitted and diffracted waves:

$$\begin{aligned} \mathbf{E}_0 &= \mathbf{e}_1 c_1(\mathbf{r}_1) \exp(i\mathbf{\kappa}_{00}\mathbf{r}_0) + \mathbf{e}_2 c_2(\mathbf{r}_1) \exp(i\mathbf{\kappa}_h\mathbf{r}_0) \\ \mathbf{\kappa}_h &= \mathbf{\kappa}_0 + \mathbf{h}, \end{aligned} \quad (58)$$

The first-order approximation with respect to  $\chi_H$  yields the inhomogeneous equation:

$$\begin{aligned} \text{rot}_0 \text{rot}_0 \mathbf{E}_1 - \kappa_{00}^2 \mathbf{E}_1 &= -(\text{rot}_1 \text{rot}_0 + \text{rot}_0 \text{rot}_1) \mathbf{E}_0 + X \mathbf{E}_0 \\ &+ \kappa^2 \left( \exp(i\mathbf{h}\mathbf{r}_0 + i\phi(\mathbf{r}_1)) + \frac{\chi_{\bar{H}}}{\chi_H} \exp(-i\mathbf{h}\mathbf{r}_0 - i\phi(\mathbf{r}_1)) \right) \mathbf{E}_0 \end{aligned} \quad (59)$$

Hence

$$\begin{aligned} \text{rot}_0 \text{rot}_0 \mathbf{E}_1 - \kappa_{00}^2 \mathbf{E}_1 &= \left( (i2(\nabla_1 c_1, \mathbf{\kappa}_{00}) + X c_1) \mathbf{e}_1 + \kappa^2 \frac{\chi_{\bar{H}}}{\chi_H} c_2 \exp(-i\phi(\mathbf{r}_1)) \right) \exp(i\mathbf{\kappa}_{00}\mathbf{r}_0) + \\ &+ (\kappa^2 c_1 \exp(i\phi(\mathbf{r}_1)) + (i2(\nabla_1 c_2, \mathbf{\kappa}_h) + X c_2) \mathbf{e}_2) \exp(i\mathbf{\kappa}_h\mathbf{r}_0) + \\ &+ \kappa^2 \frac{\chi_{\bar{H}}}{\chi_H} \exp(i(\mathbf{\kappa}_{00} - \mathbf{h})\mathbf{r}_0) \exp(-i\phi(\mathbf{r}_1)) c_1 \mathbf{e}_1 + \kappa^2 \exp(i(\mathbf{\kappa}_h + \mathbf{h})\mathbf{r}_0) \exp(i\phi(\mathbf{r}_1)) c_2 \mathbf{e}_2. \end{aligned} \quad (60)$$

Here, the gradient  $\nabla_1$  acts in the space  $\mathbf{r}_1$ . Eq. (60) was derived taking into account the additional condition  $(\nabla_1 c_1, \mathbf{e}_1) = 0$ . This indicates that the change in amplitudes on the scale  $\mathbf{r}_1$  does not violate the wave transversity.

As can easily be found from Eq. (47), two first terms in the right-hand part of Eq. (60) generate the divergence of a particular solution. The following vector system can be obtained by excluding these terms from Eq. (60):

$$\begin{cases} (i2(\nabla_1 c_1, \mathbf{\kappa}_{00}) + X c_1) \mathbf{e}_1 + \kappa^2 \frac{\chi_{\bar{H}}}{\chi_H} \exp(-i\phi(\mathbf{r}_1)) c_2 \mathbf{e}_2 = 0 \\ (i2(\nabla_1 c_2, \mathbf{\kappa}_h) + X c_2) \mathbf{e}_2 + \kappa^2 \exp(i\phi(\mathbf{r}_1)) c_1 \mathbf{e}_1 = 0 \end{cases} \quad (61)$$

According to Section 2, to satisfy the field boundedness condition, the projections of Eq. (61) on the corresponding unit vectors  $\mathbf{e}_1$  and  $\mathbf{e}_2$  must be nullified. Then, we obtain the following scalar system from Eq. (61):

$$\begin{cases} i2(\nabla_1 c_1, \mathbf{\kappa}_{00}) + Xc_1 + \kappa^2 \frac{\chi_H}{\chi_H} \eta \exp(-i\phi(\mathbf{r}_1))c_2 = 0 \\ i2(\nabla_1 c_2, \mathbf{\kappa}_h) + \kappa^2 \eta \exp(i\phi(\mathbf{r}_1))c_1 + Xc_2 = 0 \end{cases} \quad (62)$$

According to Section 2, the parameter  $X = 2(\mathbf{\kappa}_{00}\mathbf{\kappa}_{01})$  can be expressed in terms of the deviation from the exact Bragg angle  $\Delta\theta$  as follows:

$$X = \frac{\gamma_0 \kappa_{00}^2 \beta_H}{(\gamma_h - \gamma_0) \chi_H} \quad (63)$$

Eq. (62) describes the changes in the wave amplitudes on the scale  $\mathbf{r}_1$  in the Bragg reflection range for a crystal with a specified displacement field  $\mathbf{u}(\mathbf{r}_1)$ . Thus, the amplitudes are slowly varying parameters. This condition is in fact the basis of the formalism of generalized dynamic theory which results in the Takagi-Taupin equations. In this case the system of Eq. (62) should be considered a direct analog of the Takagi-Taupin equations. Let us prove this statement. We make the following substitutions in Eq. (62):

$$c_1 \rightarrow c_1 \exp(i\mathbf{a}\mathbf{r}_1), \quad c_2 \rightarrow c_2 \exp(i\mathbf{a}\mathbf{r}_1)$$

where  $\mathbf{a} = a\mathbf{n}$  is a constant vector directed along the normal to the crystal surface. Vector  $\mathbf{a}$  is chosen so as to make parameter  $X$  absent in the first equation of system (62). Then,  $a$  can be written as

$$a = \frac{X}{2\kappa_{00}\gamma_0}$$

Accordingly, Eq. (62) is reduced to the form

$$\begin{cases} i2(\nabla_1 c_1, \mathbf{\kappa}_{00}) + \kappa^2 \frac{\chi_H}{\chi_H} \eta \exp(-i\phi(\mathbf{r}_1))c_2 = 0 \\ i2(\nabla_1 c_2, \mathbf{\kappa}_h) + \kappa^2 \eta \exp(i\phi(\mathbf{r}_1))c_1 - \frac{\kappa_{00}^2 \beta_H}{\chi_H} c_2 = 0 \end{cases} \quad (64)$$

In a particular case of coplanar diffraction in the  $xz$  plane oriented normally to the crystal surface, the gradient in Eq. (64) can be written as

$$\nabla_1 = \frac{\partial}{\partial x_1} + \frac{\partial}{\partial z_1}$$

Under the assumption that the displacement field in Eq. (64) depends on only  $x$  and  $z$  coordinates in the plane of incidence, system (64) is transformed into the set of Takagi-Taupin equations written on the scale  $\mathbf{r}_1 = \chi_H \mathbf{r}$ . Thus, the formalism considered here which is based on applying the multiscale method is in complete agreement with the generalized Takagi-Taupin dynamical theory of diffraction [2]. However, there is an important difference. The reduction of the covariant theory for a deformed crystal to the Takagi-Taupin equations in a particular case suggests that key condition (57) is satisfied, i.e., this correspondence is valid for only displacement fields changing in a region comparable in size with the extinction length.

Obviously, other displacement fields which a fortiori do not satisfy condition (57) can be implemented in real crystals. In this case the use of Takagi-Taupin equations may be unjustified and in any case should be additionally analyzed.

### 3.3 Reflection coefficient

System (64) has a more general character because it was obtained without additional limitations on the Takagi-Taupin equations which is related to the rejection of the second derivatives of the field amplitudes with respect to coordinates. It is known that the boundary conditions at the crystal-vacuum interface cannot be correctly taken into account due to these limitations. Finally, the Takagi-Taupin equations cannot be applied to extremely asymmetric diffraction schemes.

Let us show how the consideration of the boundary conditions yields explicit expressions for the amplitudes of diffracted and specularly reflected waves for arbitrary angles of incidence. For simplicity we will consider diffraction in a semi-infinite crystal in the case of  $\sigma$  polarization where the vectors  $\mathbf{e}_1$  and  $\mathbf{e}_2$  are mutually parallel. Here, the solution providing extinction wave decay near the Bragg maximum should be chosen from two linearly independent solutions to Eq. (62). Correspondingly, the solution to Eq. (62) for  $c_1(\mathbf{r}_1)$  by analogy with an ideal crystal (Section 2) can be written as

$$c_1(\mathbf{r}_1) = c \exp(i\mathbf{P}(\mathbf{r}_1)\mathbf{r}_1) \quad (65)$$

where the constant  $c$  can be found from the boundary conditions and the vector  $\mathbf{P}$ , in contrast to Section 2, is assumed to be variable on the scale  $\mathbf{r}_1$ . Then, the amplitude  $c_1(\mathbf{r}_1)$  according to the first equation of system (62) is determined as

$$c_2(\mathbf{r}_1) = \frac{\chi_H}{\kappa^2 \chi_{\bar{H}}} (2(\nabla_1(\mathbf{P}\mathbf{r}_1)\mathbf{\kappa}_{00}) - X) \exp(i\mathbf{P}\mathbf{r}_1) \exp(i\phi(\mathbf{r}_1))c = \alpha c \quad (66)$$

Finally, the wave field in the semi-infinite crystal near the Bragg angle of incidence can be described by an expression that formally corresponds to an ideal crystal:

$$\mathbf{E} = \exp(i\mathbf{P}\mathbf{r}_1) (\exp(i\mathbf{\kappa}_{00}\mathbf{r}) + \alpha \exp(i\mathbf{\kappa}_h\mathbf{r}))c\mathbf{e} \quad (67)$$

The procedure of solving the boundary problem which can be reduced to a successive establishment of relations between wave amplitudes having common tangential components of the electric and magnetic fields at the crystal-vacuum interface remains the same. Therefore, one can use the expressions for amplitudes obtained in Section 2. As a result we arrive at formulas that are similar to the Fresnel formulas:

$$c = \frac{2(\mathbf{n}, \mathbf{\kappa})}{(\mathbf{n}, \mathbf{\kappa}_0 + \chi_H \mathbf{P}(\chi_H \mathbf{r}_s)) + (\mathbf{n}, \mathbf{\kappa})} c^0 \quad (68)$$

$$c_R = \frac{(\mathbf{n}\mathbf{\kappa}) - (\mathbf{n}, \mathbf{\kappa}_0 + \chi_H \mathbf{P}(\chi_H \mathbf{r}_s))}{(\mathbf{n}, \mathbf{\kappa}_0 + \chi_H \mathbf{P}(\chi_H \mathbf{r}_s)) + (\mathbf{n}\mathbf{\kappa})} c^0 \quad (69)$$

$$c_h^0 = \frac{(\mathbf{n}, \mathbf{\kappa}_h + \chi_H \mathbf{P}(\chi_H \mathbf{r}_s)) - (\mathbf{n}, \mathbf{\kappa}_{hR})}{(\mathbf{n}, \mathbf{\kappa}_h^0) - (\mathbf{n}, \mathbf{\kappa}_{hR})} \cdot \frac{2(\mathbf{n}, \mathbf{\kappa})}{(\mathbf{n}, \mathbf{\kappa}_0 + \chi_H \mathbf{P}(\chi_H \mathbf{r}_s)) + (\mathbf{n}, \mathbf{\kappa})} \alpha c^0 \quad (70)$$

The following designations are introduced here:  $\mathbf{n}$  is the unit vector directed along the normal to the crystal surface into the crystal bulk;  $\mathbf{\kappa}(c^0)$  and  $\mathbf{\kappa}_h^0(c_h^0)$  are

the wave vectors (amplitudes) of the incident and diffracted waves, respectively;  $c_R$  is the amplitude of the specularly reflected wave; and  $\mathbf{\kappa}_{hR}$  is the wave vector of the diffraction wave which is specularly reflected from the lower side of the crystal-vacuum interface. The superscript “0” is used for the parameters related to the environment. Vector  $\mathbf{r}_s$  lies in the plane of crystal-vacuum interface. In Eqs. (68)–(70), we returned to the initial dimensionless variable  $\mathbf{r}$ .

Eqs. (68)–(70) can be used to find the field amplitudes for arbitrary angles of incidence including those in the vicinity of the critical total reflection angles. In particular the formula for reflectance can be found from Eq. (70) as follows:

$$R = \left| \frac{c_h^0}{c^0} \right|^2 \cdot \frac{(\mathbf{n}\mathbf{\kappa}_h^0)}{(\mathbf{n}\mathbf{\kappa})} \quad (71)$$

In a particular case of large angles of incidence, Eq. (71) can be simplified, and Eq. (70) yields the following expression for the reflectance (which can be derived from the Takagi-Taupin equations):

$$R = \left| \frac{c_h^0}{c^0} \right|^2 \cdot \frac{(\mathbf{n}\mathbf{\kappa}_h^0)}{(\mathbf{n}\mathbf{\kappa})} = |\alpha|^2 \frac{\gamma_H}{\gamma_0} \quad (72)$$

#### 4. Conclusions

The variant of the dynamic X-ray diffraction presented in the present work is based on direct analysis of Maxwell equations for the definite model representations of the field-medium interaction taking into account the lattice presence which agree as a whole with the Ewald-Laue theory. This analysis proves to be available when the method of many scales adapted to the vector character of the problem is used. In this case the magnitude  $\chi_H$  is the parameter of expansion that corresponds in full to the physical character of the problem. This correspondence is reflected in the mathematical structure of the analyzed field equation in the crystal under conditions of dynamic scattering.

The expressions obtained for the main field characteristics in the Bragg maximum region following from the qualitative singularities of the field propagation correspond to the known results of the dynamical theory. However, the correct use of the boundary conditions leads to an expression for the reflection coefficient that substantially differs from the classical one for the case of extremely asymmetric diffraction schemes. In addition the presented approach provides the amplitude of specularly reflected wave under conditions of dynamic diffraction, which cannot be apparently obtained in the framework of traditional approaches.

In the present work, we do not state the problem to analyze the features of dynamic scattering in the sliding diffraction geometry.

In conclusion, we note the most important in our opinion differences and advantages of the approach developed in the present work.

The second-order wave equation analyzed without any additional assumptions of the possibility of the interaction of refracted and scattered waves automatically results in dynamical scattering character; in this case the kinematical scattering can be considered to a certain extent as an artificial process having limited applicability. The diffraction Laue conditions appear as a result of natural limitations of the direct expansion of the solution in the resonance case.

In the framework of the developed theory, the total consideration of different geometrical diffraction schemes including sliding geometry and other surface variants proves to be possible. In this case the order of the dispersion equations does not change. This situation is related to the effective decomposition of the problem into the construction of the uniform wave field in the crystal and the determination of field amplitudes according to the boundary conditions.

Determination of the wave field as a whole without decomposition into refracted and scattered waves is the advantage of the theory. It is clear that this feature of the theory is most important for analysis of secondary diffraction processes.

We have generalized the covariant theory of dynamic X-ray diffraction to the case of a crystal with lattice deformation. In this case the displacement field is specified, starting from model representations used in Takagi-Taupin dynamic theory. In our case (in contrast to the formalism of the Takagi-Taupin equations), lattice distortions have been taken into account on various spatial scales that were different from the scale of the lattice period.

The displacement field was also a slowly varying function of coordinates. If the displacement field is considered on one spatial scale on the order of the extinction length, then the particular case of fundamental equations for the field amplitudes is obtained as a result.

In precisely this case, we have the same result as that of the Takagi-Taupin equations. By doing so we have shown possible restrictions on the applicability of the Takagi-Taupin equations to describing dynamic diffraction in crystals using various deformation models.

At the same time, the presented theory offers an opportunity for successively taking into account displacement fields of various types implemented on different spatial scales (that are larger or significantly smaller than the extinction length).

The possibility of the correct application of boundary conditions including cases of extremely asymmetric diffraction schemes in covariant theory for ideal crystals is also wholly retained for crystals with lattice distortions. Such a situation is due to the fact that the solution of the diffraction problem proper is not related to the boundary conditions; in particular the order of fundamental equations of the theory remains the same for arbitrary diffraction geometry.

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