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CHARACTERISTIC SOLUTIONS OF TAKAGI EQUATIONS IN TWO-RAY DYNAMIC DIFFRACTION

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The earlier introduced representation of characteristic solutions of the Takagi equations in the two-ray dynamic diffraction is further developed by the authors. It is shown that this approach is physically adequate to the concept of a dynamically self-consistent system of fields in a crystal. Within the framework of this approach, equations are derived for characteristic solutions in a perfect and in a one-dimensionally distorted crystal. It is demonstrated that the system of Takagi equations involving a local accommodation function is singled out in the consideration of diffraction by one-dimensionally distorted crystals. Based on the notion of characteristic solutions of the Takagi equations, a model of a crystal with random one-dimensional distortion field is considered and the statistical averaging of the equations for characteristic solutions is carried out.

INTRODUCTION

This paper is devoted to physical justification and theory of transition to characteristic solutions [1, 2] of the Takagi equations [3] in the general case of asymmetric Bragg and Laue X-ray diffraction [4, 5] by both the perfect and the one-dimensionally distorted crystal. Attention is primarily given to the derivation and discussion of the original equations of the theory. In view of the existence of several alternative forms [3, 6] of systems of equations describing the dynamic propagation of diffraction fields in crystals, a detailed discussion of these equations appears necessary in connection with the study of diffraction phenomena in crystals with defects [7–12].

1. REPRESENTATION OF CHARACTERISTIC SOLUTIONS OF THE TAKAGI EQUATIONS

Consider the problem of two-ray dynamic X-ray diffraction (XD) by a crystal with a lattice parameter $a(z)$ varying along the z axis according to the law

$$a(z) = a(1 + \varepsilon F(z)), \tag{1}$$

where a is the lattice parameter of a perfect crystal, ε is the amplitude of the variation of the lattice parameter, and $F(z)$ is the variation function. The crystal is assumed to be a plane-parallel plate of thickness l. The z axis is directed into the plate bulk perpendicularly to its entrance surface $z = 0$.

The original system of the Takagi equations, which is obtained in the solution of the basic wave equation for the field in a crystal by the method of slowly varying amplitudes, has the following form [3] in the case of XD by a one-dimensionally distorted crystal:

$$\begin{aligned} -2i(\gamma^0/k^0)\frac{dD^0}{dz} &= \chi^0 D^0 + \chi^{-g} P D^g, \\ -2i(\gamma^g/k^0)\frac{dD^g}{dz} &= \chi^g P D^0 + (\chi^0 - \alpha) D^g + (2\gamma^g/k^0)\frac{d}{dz}(\mathbf{gu}(z)) D^g, \end{aligned} \tag{2}$$

where $D^{0,g}(z)$ are the amplitudes of the transmitted (0) and scattered (g) waves; $k^0 = 2\pi/\lambda$ is the wave vector of the wave incident on the crystal; $\gamma^{0,g} = \sin(\varphi \pm \vartheta_B)$ are the direction cosines of the wave vectors

$\mathbf{k}^0$ and $\mathbf{k}^g$, respectively (where $\mathbf{k}^g = \mathbf{k}^0 + \mathbf{g}$, g is the diffraction vector, and φ is the angle between the entrance surface of the crystal and the atomic planes in the reflecting position); $\chi^{0,\pm g}$ are the Fourier components of the polarizability of an undistorted crystal; P is the polarization factor; $\alpha = -2\sin 2\vartheta_B \Delta\vartheta$ is the accommodation proportional to the detuning $\Delta\vartheta = \vartheta - \vartheta_B$ from the refraction-uncorrected Bragg angle ϑ_B; and $\mathbf{u}(z) = \mathbf{n}a^{-1}\int_0^z (a(z') - a)\,dz'$ is the displacement function characterizing the deviation of scattering atoms from their positions in a perfect crystal ($\varepsilon = 0$), where $\mathbf{n}$ is the unit inner normal vector to the entrance surface of the crystal. In view of (1), we write the expression for the derivative of $\mathbf{u}(z)$ on the right-hand side of (2) in the form $\mathbf{g}\dfrac{d\mathbf{u}}{dz} = (\mathbf{gn})\varepsilon F(z)$. System (2) must be supplemented with the boundary conditions for the field: $D^0(0) = 1$ and $D^g(l) = 0$ in the case of the Bragg XD; $D^0(0) = 1$ and $D^g(0) = 0$ for the Laue XD.

Before proceeding to characteristic solutions [1, 2] of the Takagi equations [3] we reduce system (2), in the case of Bragg reflection, to a form symmetric with respect to the local accommodation $\alpha_B(z)$ with the aid of the transformation

$$D^{0,g}(z) = \tilde{D}^{0,g}(z)\exp\left\{-i\int_0^z \psi(z')\,dz'\right\}, \quad \psi(z) = \frac{k^0\alpha_B(z)}{4|\gamma^g|} - \frac{k^0\chi^0}{2\gamma^0};$$

$$\alpha_B(z) = \alpha_B - \frac{2|\gamma^g|}{k^0}\frac{d}{dz}(\mathbf{gu}(z)); \qquad \alpha_B = -\alpha + \chi^0(1 + |\gamma^g|/\gamma^0)$$

(the function $\alpha_B(z)$ describes the local deviation from the refraction-uncorrected Bragg angle). The amplitudes $\tilde{D}^{0,g}(z)$ satisfy the equations

$$\begin{aligned} -i\frac{d\tilde{D}^0}{dz} &= \frac{k^0\alpha_B(z)}{4|\gamma^g|}\tilde{D}^0 + \frac{\chi^{-g}Pk^0}{2\gamma^0}\tilde{D}^g, \\ i\frac{d\tilde{D}^g}{dz} &= \frac{\chi^g Pk^0}{2|\gamma^g|}\tilde{D}^0 + \frac{k^0\alpha_B(z)}{4|\gamma^g|}\tilde{D}^g. \end{aligned} \tag{3}$$

System (3) will be called the fundamental system of equations because from the very beginning it is singled out: (a) it is obtained from the exact microscopic system of Darwin recurrence relations [5, 13] and (b) the system is symmetrized with respect to the local accommodation $\alpha_B(z)$.

The physical meaning of system (3) lies in the fact that it describes the propagation along the z axis of actively (or passively, in the case of Laue diffraction) interacting fields in a system with a regular (perfect crystal) or nearly regular (slightly distorted crystal) distributed feedback.

As shown in [1, 2], in the absence of distortions ($\mathbf{u}(z) = 0$) system of equations (3) can be reduced to a system of two uncoupled first-order differential equations:

$$\frac{d\Phi_{1,2}}{dz} = \pm i\Lambda^{-1}\sqrt{\eta_B^2 - 1}\,\Phi_{1,2}, \tag{4a}$$

with the boundary conditions

$$\Phi_1(0) + \Phi_2(0) = 1, \quad (\eta_B - \sqrt{\eta_B^2 - 1})\Phi_1(l) + (\eta_B + \sqrt{\eta_B^2 - 1})\Phi_2(l) = 0, \tag{4b}$$

where $\Lambda = \dfrac{2}{k^0}\left(\dfrac{\gamma^0|\gamma^g|}{P^2\chi^g\chi^{-g}}\right)^{1/2}$ is the thickness of the primary extinction and $\eta_B = \alpha_B/(4P^2\chi^g\chi^{-g}|\gamma^g|/\gamma^0)^{1/2}$ is the angular detuning from the refraction-uncorrected Bragg angle ϑ_0 normalized to the width of the region of total reflection. In [1, 2] the functions $\Phi_{1,2}(z)$ are called characteristic solutions of the Takagi equations (3). These functions represent the amplitudes of the fields D_1 and D_2, respectively. Each of the fields is a combination of waves relating to a common propagation center on the dispersion surface [4, 5]. In contrast to the system of Takagi equations, the physical meaning of system (4a) is that it describes independent

propagation of the fields D_1 and D_2 in a perfect crystal. Therefore, Eqs. (4a) express mathematically the Ewald idea [5] of a dynamically self-consistent system of noninteracting fields in a perfect crystal.

In the case of one-dimensionally distorted crystals (ODC) ($\mathbf{u}(z) \neq 0$) the equations for the characteristic solutions have the form [1, 2]

$$\frac{d\Phi_{1,2}}{dz} = \pm i\Lambda^{-1}\sqrt{\eta_B^2 - 1}\Phi_{1,2} \mp i\frac{d}{dz}(\mathbf{gu})\{V_{1B}\Phi_1 + V_{2B}\Phi_2\} \tag{5}$$

with boundary conditions (4b), where $V_{1B,2B} = (\eta_B \mp \sqrt{\eta_B^2 - 1})/(2\sqrt{\eta_B^2 - 1})$. Equations (5) show that the presence of distortions $\mathbf{u}(z)$ in the crystal causes interaction between the propagation centers in the reciprocal space. This effect manifests itself mathematically in the fact that when $\mathbf{u}(z) \neq 0$ Eqs. (5) are coupled. It also follows from (5) that for $\mathbf{u}(z) \neq 0$ the intensities of the fields D_1 and D_2 belonging to different propagation centers on the dispersion surface are determined by the processes of rescattering of unperturbed fields between these centers, i.e., the fields D_1 and D_2 are mixed. In the Bragg diffraction the propagation centers are located on a common branch of the dispersion surface [4, 5]. By virtue of this special feature, system (5) describes intrazonal scattering of the fields.

By analogy with the Bragg XD, in the Laue XD the equations for the characteristic solutions $\Phi_{1,2}(z)$ in the general case of ODC have the form

$$\frac{d\Phi_{1,2}}{dz} = \pm i\Lambda^{-1}\sqrt{\eta_L^2 + 1}\Phi_{1,2} \pm i\frac{d}{dz}(\mathbf{gu})\{V_{1L}\Phi_1 + V_{2L}\Phi_2\} \tag{6}$$

with the boundary conditions $\Phi_{1,2}(0) = \mp V_{2L,1L}$, where

$$V_{1L,2L} = (\eta_L \pm \sqrt{\eta_L^2 + 1})/(2\sqrt{\eta_L^2 + 1}).$$

In (6) the notation $\eta_L = \alpha_L/(4P^2\chi^g\chi^{-g}\gamma^g/\gamma^0)^{1/2}$ is used for the normalized detuning from the Bragg angle ϑ_B, where $\alpha_L = -\alpha + \chi^0(1 - \gamma^g/\gamma^0)$ is the Laue accommodation. As in the Bragg case, for $\mathbf{u}(z) = 0$ system (6) splits into two uncoupled equations for the characteristic solutions $\Phi_{1,2}(z)$ (cf. (4a)). These equations describe dynamically the self-consistent fields $D_{1,2}$ that propagate independently of each other in a perfect crystal. Each of these fields is a combination of waves belonging to a common propagation center. When $\mathbf{u}(z) \neq 0$, Eqs. (6) imply that the perturbation results in interaction between the propagation centers and in mixing of the fields D_1 and D_2. The main special feature of the Laue diffraction is that the propagation centers belong to different dispersion surface branches [4]. Therefore the interaction between these centers determines the processes of interzonal scattering of the fields. Equations (6) are an analog of the well-known electron diffractometry equations, which are used in studying interzonal electron scattering by stacking faults in the Laue scheme [14].

Thus, (3) is a fundamental system in the determination of fields in both a perfect crystal and an ODC. By means of a linear transformation of diffraction fields [1] system (3) can be reduced to the equivalent system of equations (5) (or (6) in the Laue case). Note that the employed system of equations for field amplitudes in a crystal is sometimes obtained from system (2) by the exponential transformation $D^g \to D^g \exp\{i\mathbf{gu}(z)\}$ [6].

2. STATISTICAL AVERAGING OF THE SYSTEM OF DIFFERENTIAL EQUATIONS FOR CHARACTERISTIC SOLUTIONS

Within the approach of characteristic solutions of the Takagi equations, we shall consider the problem of statistical dynamic XD by a one-dimensionally distorted crystal. Assume that the lattice constant $a(z)$ varies along the z axis according to the law (cf. (1))

$$a(z) = a(1 + \mathcal{F}(z)), \tag{7}$$

where a is the lattice parameter of a perfect crystal and $\mathcal{F}(z)$ is a random function of the coordinate z. We represent the function $\mathcal{F}(z)$ in the form $\mathcal{F}(z) = E + \delta\mathcal{F}(z)$, where $E = \langle\mathcal{F}(z)\rangle$ is the regular component ($\langle\ldots\rangle$ symbolizes the statistical averaging) and $\delta\mathcal{F}(z)$ is the fluctuation component. At present there are a number of works ([7–9, 12]) where the problem of dynamic XD by crystals with defects is investigated

using the Takagi equations that are obtained from system (2) by means of the above-mentioned exponential transformation (see the remark at the end of Section 1). The parameters of the statistical XD theory based on the indicated equations are the statistical and correlation characteristics of the random function $\exp\{-i\mathbf{g}\mathbf{u}(z)\}$, such as the mean value $\langle\exp\{-i\mathbf{g}\mathbf{u}(z)\}\rangle$ (the Debye–Waller statistical factor), the correlation function, and the correlation length, where $\mathbf{u}(z)$ is the random function of defect-induced displacement of atoms from their positions in a perfect crystal.

We perform the averaging of system (5). To this end we first pass to new amplitudes $f_{1,2}(z)$ in (5) with the aid of the transformation $f_{1,2}(z) = \Phi_{1,2}(z)\exp\{\mp i\sqrt{\eta_B^2-1}\Lambda^{-1}z\}$. Using the averaging method for stochastic differential equations presented in [15] and taking into account that $\frac{d}{dz}(\mathbf{g}\mathbf{u}(z)) = (\mathbf{g}\mathbf{n})\mathcal{F}(z)$, we obtain

$$\begin{aligned}\frac{df_1^c}{dz} &= U_{1B}f_1^c + U_{2B}f_2^c\exp\{-i\Delta k_B z\},\\ \frac{df_2^c}{dz} &= -U_{2B}f_2^c - U_{1B}f_1^c\exp\{i\Delta k_B z\}\end{aligned} \tag{8}$$

($f_{1,2}^c(z) = \langle f_{1,2}(z)\rangle$ are the coherent components of the amplitudes of the characteristic solutions, $\Delta k_B = 2\Lambda^{-1}\sqrt{\eta_B^2-1}$ is the distance between the propagation centers on the dispersion surface),

$$\begin{aligned}U_{1B} &= -i(\mathbf{g}\mathbf{n})EV_{1B} - (\mathbf{g}\mathbf{n})^2V_{1B}^2\sigma^2\tau_0 - (\mathbf{g}\mathbf{n})^2V_{2B}V_{1B}\sigma^2\tau(-\Delta k_B),\\ U_{2B} &= -i(\mathbf{g}\mathbf{n})EV_{2B} - (\mathbf{g}\mathbf{n})^2V_{2B}^2\sigma^2\tau_0 - (\mathbf{g}\mathbf{n})^2V_{2B}V_{1B}\sigma^2\tau(\Delta k_B)\end{aligned}$$

($\sigma^2 = \langle(\delta\mathcal{F}(z))^2\rangle$ is the variance of the function $\mathcal{F}(z)$, $\tau(\Delta k_B) = \int_0^\infty R(y)\exp\{i\Delta k_B y\}\,dy$ is the complex correlation length, which is the Fourier transform of the correlation function $R(z-z')$ such that $\sigma^2R(z-z') = \langle\delta\mathcal{F}(z)\cdot\delta\mathcal{F}(z')\rangle$ [15], and $\tau_0 \equiv \tau(0)$). In the derivation of (8) it was assumed that $\tau_0 \lesssim \Lambda$, where Λ was the thickness of the primary extinction.

System (8) describes coherent scattering of dynamically self-consistent fields $D_{1,2}$ in a crystal with a one-dimensional random distortion field. As follows from (8), the presence of this field results in interaction of fields belonging to different propagation centers on the dispersion surface and to mixing of the coherent components $\langle D_{1,2}\rangle$ of these fields. In the case of a perfect crystal ($\mathcal{F}(z) = 0$) system (8) splits into two uncoupled equations for the amplitudes of the characteristic solutions. The parameters entering (8) are the statistical and correlation characteristics of the random function $\mathcal{F}(z)$ (7), which directly determines the distortions of the crystal lattice. Equations of similar form can also be obtained for the case of Laue diffraction.

Instead of averaging the system of equations (3) (or the equivalent system (5)), it is also possible to average the corresponding Taupin equation [16]. To derive this equation we introduce, as in [6], the complex reflection coefficient $r(z) = \left\{\frac{\chi^{-g}}{\chi^g}\frac{|\gamma^g|}{\gamma^0}\right\}^{\frac{1}{2}}\frac{D^g(z)}{D^0(z)}$, satisfying the nonlinear first-order differential equation

$$\frac{dr}{dz} + \frac{2i}{\Lambda}\alpha_B(z)r - \frac{i}{\Lambda}(1+r^2) = 0. \tag{9}$$

The introduction of the complex reflection coefficient $r(z)$ makes it possible to state the problem of diffraction by a crystal with random fluctuations of the lattice constant $a(z)$ in (7) as a Cauchy problem.

CONCLUSIONS

As is shown in the present paper, the method of characteristic solutions of the Takagi equations is consistent with the basic physical principles of the Ewald theory of dynamic diffraction. Therefore it appears natural to pass to the representation of the characteristic solutions in studying the dynamic XD. Within the framework of this approach, we considered both the Bragg and Laue diffraction schemes and derived the systems of equations (5) and (6) for the characteristic solutions $\Phi_{1,2}(z)$. In the case of a perfect crystal ($\mathbf{u}(z) = 0$), each of these systems splits into two uncoupled equations describing the dynamically self-consistent fields $D_{1,2}$ which propagate in the perfect crystal independently of each other. The field D_1 (or

D_2) combines waves belonging to a common propagation center on the dispersion surface. The presence of a distortion field $\mathbf{u}(z)$ in the crystal leads to processes of intrazonal and interzonal scattering of the fields $D_{1,2}$ in the Bragg and Laue schemes, respectively. As a result of these processes, the fields $D_{1,2}$ are mixed. In the general case of an arbitrary perturbation $\mathbf{u}(z)$ the solutions to Eqs. (5) and (6) can be found only using an approximate method, e.g., the perturbation theory method. Approximate solutions to system (5) for the case of a periodic variation function $F(z)$ in (1) (a superlattice) were obtained in [1, 2]. A system similar to (6) was used in [17] in an analysis of the Laue XD by a thick absorbing crystal distorted by an ultrasonic wave under a resonance condition: $\lambda_s \simeq \Lambda$, where λ_s is the ultrasound wavelength.

Thus, we have considered the basic systems of equations describing the propagation of diffraction fields in crystals with deterministic (or random) distortion fields. The latter are not related to the introduction of the displacement function $\mathbf{u}(z)$ but depend on the variation function $F(z)$ in (1) (or $\mathcal{F}(z)$ in (7)), which directly determines the distortions of the crystal lattice parameter $a(z)$ in (1) (or in (7)).

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