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Statistical dynamical theory of X-ray diffraction in the Bragg case: application to triple-crystal diffractometry

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The statistical dynamical theory of X-ray diffraction is developed for a crystal containing statistically distributed microdefects. Fourier-component equations for coherent and diffuse (incoherent) scattered waves have been obtained in the case of so-called triple-crystal diffractometry. New correlation lengths and areas are introduced for characterization of the scattered volume.

1. Introduction

The statistical dynamical diffraction theory (SDDT) formulated first by Kato (1980*a*,*b*) is the general approach to the description of the X-ray scattering by a crystal with randomly distributed defects. Various authors (Becker & Al Haddad, 1989, 1990; Guigay, 1989; Guigay & Chukhovskii, 1992, 1995) have obtained further modifications of the original Kato treatment (Kato, 1980*a*,*b*).

Kato (1991) has proposed an approach based upon the Green-function concept. In its original form, which is free from the so-called Takagi–Taupin approximation, this theory is too complex for practical applications. All above-mentioned formulations of the SDDT have been developed for a point source in Laue geometry (the case of a spherical wave).

Holý (Holý, 1982*a*,*b*; Holý & Gabrielyan, 1987) developed an alternative approach to SDDT based upon the mutual coherency function. This approach was used (Holý & Kubena, 1992; Holý *et al*., 1992, 1993, 1994; Darhuber *et al.*, 1997) for the calculation of the distribution of diffuse scattered waves within the framework of the kinematical diffraction theory (Dederichs, 1971; Krivoglaz, 1996).

The X-ray diffraction theory of plane waves is more important for practical purposes, since it takes into account the angular distribution of the scattering intensity. Bushuev (1989*a*,*b*) offered such a SDDT within the framework of Kato's treatment (Kato, 1980*a*,*b*). Punegov (1990) developed the equations of SDDT for heteroepitaxial systems non-uniform in depth. In our comment (Pavlov & Punegov, 1997), we noted that Chinese scientists (An *et al.*, 1995) have formulated this approach anew. Pavlov & Punegov (1998*a*,*b*) have obtained the most general equations of SDDT for a deformed crystal in the case of plane waves. Recently, Guigay & Vartanyants (1999) have developed SDDT for large correlation lengths.

The statistical theory of X-ray diffraction by non-uniform and multilayer systems (Punegov, 1991*a*, 1993, 1994) has been used for solving inverse problems of X-ray diffraction in cases of laser heterostructures (Pavlov *et al*., 1995) and non-uniform epitaxial layers with linear change of components with depth (Punegov *et al*., 1996). Both the double- and the triple-crystal diffractometry data must be allowed for the inverse problem solving within the framework of the statistical theory of X-ray diffraction. Using only double-crystal diffractometry data (An *et al.*, 1995; Li *et al.*, 1995) does not enable one to obtain reliable information on the structural characteristics of epitaxial layers, since the scattering intensity involves both the coherent and the diffuse components (Punegov, 1991*b*).

High-resolution triple-crystal diffractometry (Iida & Kohra, 1979; Zaumseil & Winter, 1982*a*,*b*; Lomov *et al*., 1985) gives much more information about investigated structures with defects than double-crystal diffractometry. However, to date, any approach of Kato's variant of SDDT applied to triple-crystal diffractometry has not been developed.

It should be noted that Bushuev (1988) has applied the double-crystal diffractometry approach of SDDT to calculate the triple-crystal diffractometry. He has modernized the expression of the correlation length from $\tau(\omega)$ to $\tau(\omega, \varepsilon)$, where ω is the angular deviation of a sample and ε is the angular deviation of an analyser crystal. However, such an approach is a very strong semi-empirical simplification.

This paper aims to develop the equations of SDDT presented in Pavlov & Punegov (1998*a*,*b*) for the case of triple-crystal diffractometry.

The organization of this paper is as follows. In §2, we develop the theoretical formalism for X-ray dynamical diffraction using the Fourier transform. In particular, we obtain an integral solution for the Fourier components of the diffracted and transmitted wavefields. §3 examines the

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coherent wavefield within a crystal, including the case of a semi-infinite crystal. §4 discusses the diffuse wavefield. Finally, in §5, we present our concluding remarks.

2. Theoretical formalism for the Fourier components of the wavefield

We consider dynamical X-ray diffraction in Bragg geometry from a crystal containing statistically distributed defects. The diffraction geometry and the parameters are shown in Fig. 1. A monochromatic wave emanating from a monochromator is incident on the entrance surface of the crystal, which is shaped like a homogeneous crystalline layer with thickness l. This layer has large extent in the direction of the axis X. The incident divergent beam is restricted in both the X and Y directions by using vertical and horizontal slits between the monochromator and the crystal. We use the oblique coordinates, S_0 and S_H (see Fig. 1), with unit vectors $\mathbf{s}_0 = \mathbf{K}_0/|\mathbf{K}_0|$ and $\mathbf{s}_H = \mathbf{K}_H/|\mathbf{K}_H|$.

The relationships between the oblique coordinates, S_0 and S_H, and the Cartesian ones, X and Z, with the X axis oriented along the crystal surface and the Z axis oriented into the crystal (Pavlov & Punegov, 1998*a*,*b*), are:

$$\begin{cases} x = s_0\cos(\theta_B - \varphi) + s_h\cos(\theta_B + \varphi) \\ z = s_0\sin(\theta_B - \varphi) - s_h\sin(\theta_B + \varphi), \end{cases} \tag{1}$$

θ_B is the Bragg angle. These relationships can be rewritten using the asymmetry factor

$$b = \frac{\sin(\theta_B - \varphi)}{\sin(\theta_B + \varphi)} = \frac{\sin(\theta_1)}{\sin(\theta_2)}$$

(see Fig. 1):

$$s_0 - \frac{s_h}{b} = \frac{z}{\sin\theta_1}; \quad bs_0 - s_h = \frac{z}{\sin\theta_2}. \tag{2}$$

Inside the crystal, the X-ray wavefield is described by a system of equations of dynamical diffraction (Takagi, 1969; Taupin, 1964; Afanas'ev & Kohn, 1971):

$$\begin{cases} \dfrac{\partial E_0}{\partial s_0} = \dfrac{i\pi}{\lambda}E_0\chi_0 + \dfrac{i\pi}{\lambda}\chi_{\bar h}C\exp(i\mathbf{h}\cdot\delta\mathbf{u})E_h \\ \dfrac{\partial E_h}{\partial s_h} = \dfrac{i\pi}{\lambda}E_h(\chi_0 - \alpha_h) + \dfrac{i\pi}{\lambda}\chi_h C\exp(-i\mathbf{h}\cdot\delta\mathbf{u})E_0. \end{cases} \tag{3}$$

Here, E_0 and E_h are the amplitudes of the transmitted and diffracted waves, $\alpha_h = -2\sin 2\theta_B\omega$, $\omega = \theta - \theta_B$ is the deviation angle of the investigated crystal from the Bragg position, $\mathbf{h}$ is the diffraction vector, $\chi_{0,h,\bar h}$ are the Fourier components of the susceptibility, λ is the X-ray wavelength, C is the polarization factor,

$$C = \begin{cases} 1 & \sigma\text{ polarization} \\ \cos(2\theta_B) & \pi\text{ polarization,} \end{cases}$$

and $\delta\mathbf{u}$ is the atomic displacement vector caused by statistically distributed defects.

In the system of equations (3), we perform the following substitution (Pavlov & Punegov, 1998*a*,*b*):

$$\begin{cases} \tilde E_0 = E_0\exp[-(i\pi/\lambda)\chi_0(s_0 - s_h/b)] \\ \quad = E_0\exp[-(i\pi/\lambda)\chi_0(z/\sin\theta_1)] \\ \tilde E_h = E_h\exp[-(i\pi/\lambda)(\chi_0 - \alpha_h)(s_h - s_0 b)] \\ \quad = E_h\exp[(i\pi/\lambda)(\chi_0 - \alpha_h)(z/\sin\theta_2)]. \end{cases} \tag{4}$$

Thereafter, the system of equations (3) can be rewritten in the form

$$\begin{cases} \dfrac{\partial \tilde E_0(s_0,s_h)}{\partial s_0} = \dfrac{i\pi}{\lambda}\chi_{\bar h}C\exp(i\mathbf{h}\cdot\delta\mathbf{u})\tilde E_h(s_0,s_h) \\ \qquad\times\exp\left\{\dfrac{i\pi}{\lambda}\left(\dfrac{s_h}{b} - s_0\right)[\chi_0(1+b) - b\alpha_h]\right\} \\ \dfrac{\partial \tilde E_h(s_0,s_h)}{\partial s_h} = \dfrac{i\pi}{\lambda}\chi_h C\exp(-i\mathbf{h}\cdot\delta\mathbf{u})\tilde E_0(s_0,s_h) \\ \qquad\times\exp\left\{\dfrac{i\pi}{\lambda}\left(s_0 - \dfrac{s_h}{b}\right)[\chi_0(1+b) - b\alpha_h]\right\}, \end{cases} \tag{5}$$

which allows an integral solution for $\tilde E_{0,h}$ to be obtained:

$$\begin{aligned} \tilde E_0(s_0,s_h) = \tilde E_0(\hat s_0,\hat s_h) &+ i\frac{\pi}{\lambda}C\int_{\hat s_0}^{s_0}\chi_{\bar h}\exp[i\mathbf{h}\cdot\delta\mathbf{u}(s_0',s_h)] \\ &\times\exp\left\{i\frac{\pi}{\lambda}\left(\frac{s_h}{b} - s_0'\right)[\chi_0(1+b) - b\alpha_h]\right\} \\ &\times\tilde E_h(s_0',s_h)\,\mathrm{d}s_0' \end{aligned} \tag{6a}$$

$$\begin{aligned} \tilde E_h(s_0,s_h) = \tilde E_h(\bar s_0,\bar s_h) &+ i\frac{\pi}{\lambda}C\int_{\bar s_h}^{s_h}\chi_h\exp[-i\mathbf{h}\cdot\delta\mathbf{u}(s_0,s_h')] \\ &\times\exp\left\{i\frac{\pi}{\lambda}\left(s_0 - \frac{s_h'}{b}\right)[\chi_0(1+b) - b\alpha_h]\right\} \\ &\times\tilde E_0(s_0,s_h')\,\mathrm{d}s_h'. \end{aligned} \tag{6b}$$

We define the boundary conditions as follows:

$$\begin{aligned} E_0(z=0 \Leftrightarrow (\hat s_0,\hat s_h)) &= E_0^{(\mathrm{in})}(x,0) \\ E_h(z=l \Leftrightarrow (\bar s_0,\bar s_h)) &= 0. \end{aligned} \tag{7}$$

Here, $E_0^{(\mathrm{in})}(x,0)$ is the amplitude of the incident wave on the entrance surface. In comparison with our previous article (Pavlov & Punegov, 1998*a*,*b*), we take into account the general case of the inhomogeneous pseudo-plane incident wave. In the rectangular coordinates (see Fig. 1), these solutions (6*a*), (6*b*) can be rewritten as

$$\begin{aligned} \tilde E_0(x,z) = \tilde E_0(x - z\cot\theta_1, 0) &+ i\int_0^z a_{\bar h}\exp[i\mathbf{h}\cdot\delta\mathbf{u}(x + (z'-z)\cot\theta_1, z')] \\ &\times\exp(-i\eta z')\tilde E_h(x + (z'-z)\cot\theta_1, z')\,\mathrm{d}z' \end{aligned} \tag{8a}$$

$$\begin{aligned} \tilde E_h(x,z) = \tilde E_h(x - (l-z)\cot\theta_2, l) &+ i\int_z^l a_h\exp[-i\mathbf{h}\cdot\delta\mathbf{u}(x - (z'-z)\cot\theta_2, z')] \\ &\times\exp(i\eta' z')\tilde E_0(x - (z'-z)\cot\theta_2, z')\,\mathrm{d}z', \end{aligned} \tag{8b}$$

where

$$\eta' = \frac{\pi}{\lambda \sin\theta_1}[(1+b)\chi_0 + 2b\omega\sin(2\theta_B)];$$
$$a_0 = \frac{\pi\chi_0}{\lambda\sin\theta_1}; \quad a_h = \frac{\pi\chi_h C}{\lambda\sin\theta_2}; \quad a_{\bar h} = \frac{\pi\chi_{\bar h} C}{\lambda\sin\theta_1}. \qquad (9)$$

The amplitudes of the plane waves $\tilde{E}_0(x, z)$ and $\tilde{E}_h(x, z)$ inside the crystal can be represented by the appropriate Fourier integrals. Deviation vectors $\mathbf{q}_0$ and $\mathbf{q}_h$ are perpendicular to the average wave vectors $\mathbf{K}_0$ and $\mathbf{K}_H$, respectively (see Appendix *A* and Fig. 1):

$$\tilde{E}_0(x,z) = (1/2\pi)\int \mathrm{d}q_{0_x}\, \tilde{E}_0(q_{0_x}, z)\exp(iq_{0_x}x) \qquad (10a)$$
$$\tilde{E}_h(x,z) = (1/2\pi)\int \mathrm{d}q_{h_x}\, \tilde{E}_h(q_{h_x}, z)\exp(iq_{h_x}x). \qquad (10b)$$

The inverse Fourier transformation offers the amplitude of the plane waves propagating in the ($\mathbf{K}_0$ + $\mathbf{q}_0$) and ($\mathbf{K}_H$ + $\mathbf{q}_\mathrm{h}$) directions, respectively.

$$\tilde{E}_0(q_{0_x}, z) = \int \mathrm{d}x\, \tilde{E}_0(x,z)\exp(-iq_{0_x}x) \qquad (11a)$$
$$\tilde{E}_h(q_{h_x}, z) = \int \mathrm{d}x\, \tilde{E}_h(x,z)\exp(-iq_{h_x}x). \qquad (11b)$$

Usually, in experiment the intensity is integrated along the *Y* coordinate by the detector. Therefore, we do not take the Fourier transformation along the *Y* axis.

In the formal solutions (8*a*), (8*b*), we substitute the Fourier representation (10*a*), (10*b*). In addition, using (11*a*), (11*b*), we take the inverse Fourier transformation of the obtained expressions and return to the initial representation of the wavefield amplitudes:

$$\begin{aligned} E_0(q_{0_x}, z) &= E_0(q_{0_x}, 0)\exp(-iq_{0_x} z\cot\theta_1)\exp(ia_0 z) \\ &\quad + i\int \mathrm{d}x\, \exp(-iq_{0_x}x)\exp(ia_0 z) \\ &\quad \times \int_0^z \mathrm{d}z'\, a_{\bar h}\exp[i\mathbf{h}\cdot\delta\mathbf{u}(x + (z'-z)\cot\theta_1, z')] \\ &\quad \times E_h(x + (z'-z)\cot\theta_1, z')\exp(-ia_0 z') \qquad (12a) \end{aligned}$$

$$\begin{aligned} E_h(q_{h_x}, z) &= E_h(q_{h_x}, l)\exp[-iq_{h_x}(l-z)\cot\theta_2] \\ &\quad \times \exp[i(\eta' - a_0)(l-z)] + i\int \mathrm{d}x\, \exp(-iq_{h_x}x) \\ &\quad \times \int_z^l \mathrm{d}z'\, a_h\exp[-i\mathbf{h}\cdot\delta\mathbf{u}(x - (z'-z)\cot\theta_2, z')] \\ &\quad \times \exp[i(\eta' - a_0)(z'-z)]E_0(x - (z'-z)\cot\theta_2, z'). \qquad (12b) \end{aligned}$$

Here we have used the well known expression for the Dirac δ function:

$$\delta(q - q') = (1/2\pi)\int \mathrm{d}x\, \exp[i(q-q')x]. \qquad (13)$$

Thereafter, we take the Fourier transformation of the wave fields in integrals in (12*a*), (12*b*) and assume the following boundary conditions of the X-ray diffraction in the Bragg case: on the entrance surface, $E_0^{(\mathrm{in})}(q_{0_x}) = E_0(q_{0_x}, 0)$, and, on the bottom boundary of the crystal, $E_h(q_{h_x}, l) = 0$. These boundary conditions follow as a result of the Fourier transformation of (7). Finally, we obtain the formal solution for the wavefields in the directions ($\mathbf{K}_0$ + $\mathbf{q}_0$) and ($\mathbf{K}_H$ + $\mathbf{q}_h$), respectively:

$$\begin{aligned} E_0(q_{0_x}, z) &= E_0(q_{0_x}, 0)\exp[-i(q_{0_x}\cot\theta_1 - a_0)z] \\ &\quad + (i/2\pi)\int \mathrm{d}x\, \exp(-iq_{0_x}x) \\ &\quad \times \int_0^z \mathrm{d}z'\, a_{\bar h}\exp[i\mathbf{h}\cdot\delta\mathbf{u}(x + (z'-z)\cot\theta_1, z')] \\ &\quad \times \exp[-ia_0(z'-z)]\int \mathrm{d}q_{h_x}\, E_h(q_{h_x}, z') \\ &\quad \times \exp\{iq_{h_x}[x + (z'-z)\cot\theta_1]\} \qquad (14a) \end{aligned}$$

$$\begin{aligned} E_h(q_{h_x}, z) &= (i/2\pi)\int \mathrm{d}x\, \exp(-iq_{h_x}x) \\ &\quad \times \int_z^l \mathrm{d}z'\, a_h\exp[-i\mathbf{h}\cdot\delta\mathbf{u}(x - (z'-z)\cot\theta_2, z')] \\ &\quad \times \exp[i(z'-z)(\eta' - a_0)]\int \mathrm{d}q_{0_x}\, E_0(q_{0_x}, z') \\ &\quad \times \exp\{iq_{0_x}[x - (z'-z)\cot\theta_2]\}. \qquad (14b) \end{aligned}$$

Equations (14*a*), (14*b*) describe the complex process of interactions between the Fourier components of the waves, including the coherent and the diffuse parts.

3. Coherent wavefields

There are three types of X-ray diffraction in crystals. If the crystal lattice is free from randomly distributed defects, then the X-ray diffraction is completely coherent. If the crystal lattice is partially damaged by statistically distributed microdefects, then waves scattered coherently and diffusely are formed. If the whole crystal bulk consists of blocks whose size is less than the extinction length and these blocks are rotated relative to each other by small angles (short-range order), then the X-ray scattering in such a crystal is total incoherent. We consider the second variant as the general case.

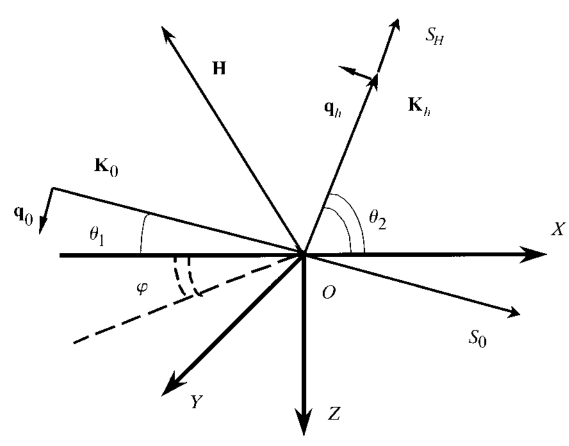

Figure 1
The diffraction geometry is shown in this figure, where $\mathbf{K}_0$ is the average wavevector of the incident wave, $\mathbf{K}_h$ is the average wavevector of the diffracted wave. $\mathbf{H}$ is the diffraction vector and φ is the inclination of the lattice planes with respect to the crystal surface (*X* axis). The vectors $\mathbf{K}_0$, $\mathbf{K}_h$ and $\mathbf{H}$ lie within the plane of diffraction (*XOZ*). The *Y* axis is oriented perpendicular to the diffraction plane and lies on the crystal surface. S_0 and S_h are the axes of the oblique coordinates (S_0, S_h). $\mathbf{q}_0$ and $\mathbf{q}_h$ are the deviation vectors.

After some algebra, we write equations (5) in rectangular coordinates:

$$\begin{cases} \dfrac{\partial \tilde{E}_0(q_{0_x}, z)}{\partial z} = -iq_{0_x} \cot\theta_1 \tilde{E}_0(q_{0_x}, z) \\ \qquad + \dfrac{i}{2\pi} \displaystyle\int \mathrm{d}x\, a_{\bar{h}} \exp(-iq_{0_x} x) \exp[i\mathbf{h}\cdot\delta\mathbf{u}(x,z)] \\ \qquad \times \exp(-i\eta' z) \displaystyle\int \mathrm{d}q_{h_x} \exp(iq_{h_x} x) \tilde{E}_h(q_{h_x}, z) \\ \dfrac{\partial \tilde{E}_h(q_{h_x}, z)}{\partial z} = iq_{h_x} \cot\theta_2 \tilde{E}_h(q_{h_x}, z) \\ \qquad - \dfrac{i}{2\pi} \displaystyle\int \mathrm{d}x\, a_h \exp(-iq_{h_x} x) \\ \qquad \times \exp[-i\mathbf{h}\cdot\delta\mathbf{u}(x,z)] \exp(i\eta' z) \\ \qquad \times \displaystyle\int \mathrm{d}q_{x_0} \exp(iq_{0_x} x) \tilde{E}_0(q_{0_x}, z). \end{cases} \quad (15)$$

By the statistical averaging of (15), we take into account two components of the phase factor:

$$\exp(i\mathbf{h}\cdot\delta\mathbf{u}) = \Phi = \langle\Phi\rangle + \delta\Phi = f + \delta\Phi. \quad (16)$$

In the original Kato (1980*a*,*b*) treatment, the static Debye–Waller factor was denoted as E. In all our previous articles, we have used only this designation. However, the same letter designating the wave amplitudes causes difficulties in the reading of the paper. Therefore, following Bushuev (1994), we use the designation f for the static Debye–Waller factor. Using the formal solutions (12*a*), (12*b*), we write the statistical averaging of the equations (15) for the initial amplitudes:

$$\begin{aligned} \frac{\partial E_0^c(q_{0_x}, z)}{\partial z} &= i(a_0 - q_{0_x}\cot\theta_1) E_0^c(q_{0_x}, z) \\ &+ \frac{i}{2\pi}\iint \mathrm{d}q_{h_x}\,\mathrm{d}x\, a_{\bar{h}} f \exp[i(q_{h_x} - q_{0_x})x] E_h^c(q_{h_x}, z) \\ &- \frac{1}{(2\pi)^2}\iiint \mathrm{d}\tilde{q}_{0_x}\,\mathrm{d}q_{h_x}\,\mathrm{d}x\, a_h a_{\bar{h}} E_0^c(\tilde{q}_{0_x}, z) \\ &\times \exp[-i(q_{0_x} - \tilde{q}_{0_x})x] \\ &\times \int \mathrm{d}\tilde{x} \exp[i(q_{h_x} - \tilde{q}_{0_x})(x - \tilde{x})] \\ &\times \int_z^l \mathrm{d}z' \langle \delta\Phi(x,z)\delta\Phi^*(\tilde{x} - (z'-z)\cot\theta_2, z')\rangle \\ &\times \exp[i(z'-z)\eta'] \exp[-i\tilde{q}_{0_x}(z'-z)\cot\theta_2] \end{aligned} \quad (17a)$$

$$\begin{aligned} \frac{\partial E_h^c(q_{h_x}, z)}{\partial z} &= i(a_0 - \eta' + q_{h_x}\cot\theta_2) E_h^c(q_{h_x}, z) \\ &- \frac{i}{2\pi}\iint \mathrm{d}q_{0_x}\,\mathrm{d}x\, a_h f \exp[i(q_{0_x} - q_{h_x})x] E_0^c(q_{0_x}, z) \\ &+ \frac{1}{(2\pi)^2}\iiint \mathrm{d}\tilde{q}_{h_x}\,\mathrm{d}q_{0_x}\,\mathrm{d}x\, a_h a_{\bar{h}} E_h^c(\tilde{q}_{h_x}, z) \\ &\times \exp[-i(q_{h_x} - \tilde{q}_{h_x})x] \\ &\times \int \mathrm{d}\tilde{x} \exp[i(q_{0_x} - \tilde{q}_{h_x})(x - \tilde{x})] \\ &\times \int_0^z \mathrm{d}z' \langle \delta\Phi^*(x,z)\delta\Phi(\tilde{x} + (z'-z)\cot\theta_1, z')\rangle \\ &\times \exp[-i(z'-z)\eta'] \exp[i\tilde{q}_{h_x}(z'-z)\cot\theta_1]. \end{aligned} \quad (17b)$$

Here, $E_{0,h}^c(q, z) = \langle E_{0,h}(q, z)\rangle$ are the amplitudes of the coherent wave. We assume that the amplitudes of the coherent wave slowly change with the linear sizes of the defects. Hence, these amplitudes $\tilde{E}_{0,h}^c$ change more slowly than $\delta\Phi$ and we can neglect the correlation $\langle\delta\Phi\tilde{E}_{0,h}^c\rangle$. In other words, the mean sizes of the statistically distributed defects are less than the extinction length.

Following the treatment of Kato's SDDT (Kato, 1980*a*,*b*), the differential correlation areas can be given in the form

$$\begin{aligned} \hat{\tau}_1^c &= [1/(1-f^2)] \textstyle\int \mathrm{d}\varepsilon \exp[-i(q_{h_x} - q_{0_x})\varepsilon] \\ &\times \int_0^{l-z\approx\infty} \mathrm{d}\xi \exp[i\xi(\eta' - q_{0_x}\cot\theta_2)] \\ &\times \langle\delta\Phi(x,z)\delta\Phi^*(x + \varepsilon - \xi\cot\theta_2, z + \xi)\rangle \end{aligned} \quad (18)$$

$$\begin{aligned} \hat{\tau}_2^c &= [1/(1-f^2)] \textstyle\int \mathrm{d}\rho \exp[-i(q_{0_x} - q_{h_x})\rho] \\ &\times \int_0^{z\approx\infty} \mathrm{d}\psi \exp[i\psi(\eta' - q_{h_x}\cot\theta_1)] \\ &\times \langle\delta\Phi^*(x,z)\delta\Phi(x + \rho - \psi\cot\theta_1, z - \psi)\rangle. \end{aligned} \quad (19)$$

These differential correlation areas are functions of angular parameters only in the case of uniform distribution of small size defects. Using (18) and (19), the equations for the coherent amplitudes can be rewritten in the form

$$\begin{cases} \dfrac{\partial E_0^c(q_{0_x}, z)}{\partial z} = i(a_0 - q_{0_x}\cot\theta_1) E_0^c(q_{0_x}, z) \\ \qquad + \dfrac{i}{2\pi}\displaystyle\iint \mathrm{d}q_{h_x}\,\mathrm{d}x\, a_{\bar{h}} f \exp[i(q_{h_x} - q_{0_x})x] \\ \qquad \times E_h^c(q_{h_x}, z) - \dfrac{1}{(2\pi)^2}\displaystyle\iiint \mathrm{d}\tilde{q}_{0_x}\,\mathrm{d}q_{h_x}\,\mathrm{d}x\, a_h a_{\bar{h}} \\ \qquad \times (1-f^2) E_0^c(\tilde{q}_{0_x}, z) \exp[-i(q_{0_x} - \tilde{q}_{0_x})x]\hat{\tau}_1^c \\ \dfrac{\partial E_h^c(q_{h_x}, z)}{\partial z} = i(a_0 - \eta' + q_{h_x}\cot\theta_2) E_h^c(q_{h_x}, z) \\ \qquad - \dfrac{i}{2\pi}\displaystyle\iint \mathrm{d}q_{0_x}\,\mathrm{d}x\, a_h f \exp[i(q_{0_x} - q_{h_x})x] \\ \qquad \times E_0^c(q_{0_x}, z) \\ \qquad + \dfrac{1}{(2\pi)^2}\displaystyle\iiint \mathrm{d}\tilde{q}_{h_x}\,\mathrm{d}q_{0_x}\,\mathrm{d}x\, a_h a_{\bar{h}} (1-f^2) \\ \qquad \times E_h^c(\tilde{q}_{h_x}, z) \exp[-i(q_{h_x} - \tilde{q}_{h_x})x]\hat{\tau}_2^c. \end{cases} \quad (20)$$

In the first equation of the system (20), the correlation area $\hat{\tau}_1^c$ can be integrated over the deviation q_{h_x} and, in the second equation, the correlation area $\hat{\tau}_2^c$ can be integrated over deviation q_{0_x}, thus we obtain the integrated correlation lengths:

$$\bar{\tau}_1^c = (1/2\pi)\int \mathrm{d}q_{h_x}\,\hat{\tau}_1^c$$
$$= [1/(1-f^2)]\int_0^{l-z\approx\infty} \mathrm{d}\xi\,\exp[i\xi(\eta' - q_{0_x}\cot\theta_2)]$$
$$\times\langle\delta\Phi(x,z)\delta\Phi^*(x-\xi\cot\theta_2, z+\xi)\rangle \quad (21)$$
$$\bar{\tau}_2^c = (1/2\pi)\int \mathrm{d}q_{0_x}\,\hat{\tau}_2^c$$
$$= [1/(1-f^2)]\int_0^{z\approx\infty} \mathrm{d}\psi\,\exp[i\psi(\eta' - q_{h_x}\cot\theta_1)]$$
$$\times\langle\delta\Phi^*(x,z)\delta\Phi(x-\psi\cot\theta_1, z-\psi)\rangle. \quad (22)$$

If the incident wave is a plane wave (all components with non-zero q_0 are equal to zero) and the registration system works in the so-called θ–2θ mode ($q_h = 0$), then the integrated correlation lengths are identical to the correlation lengths [equations (13), (14)] in our previous paper (Pavlov & Punegov 1998*a*,*b*).

Finally, the system of differential equations for the coherent amplitudes is given as

$$\begin{cases} \dfrac{\partial E_0^c(q_{0_x},z)}{\partial z} = i(a_0 - q_{0_x}\cot\theta_1)E_0^c(q_{0_x},z) + ia_{\bar{h}}fE_h^c(q_{0_x},z) \\ \qquad - \dfrac{1}{2\pi}a_h a_{\bar{h}}(1-f^2)\displaystyle\iint \mathrm{d}\tilde{q}_{0_x}\,\mathrm{d}x\,E_0^c(\tilde{q}_{0_x},z) \\ \qquad \times\exp[-i(q_{0_x}-\tilde{q}_{0_x})x]\bar{\tau}_1^c \\ \dfrac{\partial E_h^c(q_{h_x},z)}{\partial z} = i(a_0 - \eta' + q_{h_x}\cot\theta_2)E_h^c(q_{h_x},z) \\ \qquad - ia_h fE_0^c(q_{h_x},z) + \dfrac{1}{2\pi}a_h a_{\bar{h}}(1-f^2) \\ \qquad \times\displaystyle\iint \mathrm{d}\tilde{q}_{h_x}\,\mathrm{d}x\,E_h^c(\tilde{q}_{h_x},z) \\ \qquad \times\exp[-i(q_{h_x}-\tilde{q}_{h_x})x]\bar{\tau}_2^c. \end{cases} \quad (23)$$

Here, we assume that defects are uniformly distributed in the direction of the X axis. Then the correlation lengths can be taken out of the integral:

$$\begin{cases} \dfrac{\partial E_0^c(q_{0_x},z)}{\partial z} = i(a_0 - q_{0_x}\cot\theta_1)E_0^c(q_{0_x},z) + ia_{\bar{h}}fE_h^c(q_{0_x},z) \\ \qquad - a_h a_{\bar{h}}(1-f^2)\bar{\tau}_1^c E_0^c(q_{0_x},z) \\ \dfrac{\partial E_h^c(q_{h_x},z)}{\partial z} = i(a_0 - \eta' + q_{h_x}\cot\theta_2)E_h^c(q_{h_x},z) \\ \qquad - ia_h fE_0^c(q_{h_x},z) + a_h a_{\bar{h}}(1-f^2)\bar{\tau}_2^c E_h^c(q_{h_x},z). \end{cases} \quad (24)$$

Since the tangential projections of the wavevectors are identical for coherent components E_0^c and E_h^c, the Fourier component $E_0^c(q_{0_x},z)$ corresponds to the Fourier component $E_h^c(q_{h_x},z)$, where $q_{h_x}\equiv q_{0_x}$. Then analytical solutions of the system of equations (24) can be written as

$$E_0^c(q_{0_x},z) = A_1\exp[i(\lambda_0+\lambda_1)z] + A_2\exp[i(\lambda_0-\lambda_1)z]$$
$$E_h^c(q_{0_x},z) = k_1A_1\exp[i(\lambda_0+\lambda_1)z] + k_2A_2\exp[i(\lambda_0-\lambda_1)z], \quad (25)$$

where

$$a_1 = i(a_0 - q_{0_x}\cot\theta_1) - a_h a_{\bar{h}}(1-f^2)\bar{\tau}_1^c;\quad a_2 = ia_{\bar{h}}f;$$
$$a_3 = -ia_hf;\quad a_4 = i(a_0 - \eta' + q_{0_x}\cot\theta_2) + a_h a_{\bar{h}}(1-f^2)\bar{\tau}_2^c \quad (26)$$

and

$$(\lambda_0\pm\lambda_1) = -\frac{i}{2}\{a_1 + a_4 \pm [(a_1+a_4)^2 - 4(a_1a_4 - a_2a_3)]^{1/2}\}. \quad (27)$$

To obtain coefficients $k_{1,2}$, the general solution (25) should be substituted into the differential equations (24).

$$k_1 = 2a_3/\{a_1 - a_4 + [(a_1+a_4)^2 - 4(a_1a_4 - a_2a_3)]^{1/2}\};$$
$$k_2 = 2a_3/\{a_1 - a_4 - [(a_1+a_4)^2 - 4(a_1a_4 - a_2a_3)]^{1/2}\}. \quad (28)$$

The coefficients $A_{1,2}$ can be obtained from conditions in the boundary. Since the Fourier components of the coherent amplitude are independent of each other, their calculations can be made for each Fourier component separately.

3.1. Semi-infinite crystal

By consideration of the X-ray diffraction in a semi-infinite crystal, we take into account that only one of two components for each wave should remain in the analytical solution (25). Choosing between them is based upon the condition that the intensity of the penetrating wave should be decreased inside the semi-infinite crystal. Therefore, the condition $\mathrm{Im}(\lambda_0\pm\lambda_1) > 0$ can be used as a basic guideline in deciding which component of the wave to employ. Also, it is possible to neglect the term containing the correlation length. The modified coefficients (26) are

$$\bar{a}_1 = i(a_0 - q_{0_x}\cot\theta_1);\quad \bar{a}_2 = ia_{\bar{h}}f;$$
$$a_3 = -ia_hf;\quad \bar{a}_4 = i(a_0 - \eta' + q_{0_x}\cot\theta_2). \quad (29)$$

The reflection coefficient for any Fourier component of the coherent wave can be written as

$$R_s = (1/b^{1/2})k_{1,2}, \quad (30)$$

where the rule of choosing between the coefficients $k_{1,2}$ is the same as the above-mentioned procedure for determination of the sign in the exponent of the analytical solution (25).

4. Diffuse wavefields

We consider a yield of the diffuse scattered waves within the framework of SDDT. The intensities of the diffuse waves are differences between the total intensities and the coherent intensities:

$$I_{0,h}^d(q_x,z) = \langle E_{0,h}(q_x,z)E_{0,h}^*(q_x,z)\rangle - \langle E_{0,h}(q_x,z)\rangle\langle E_{0,h}^*(q_x,z)\rangle. \quad (31)$$

Derivation of the equations for the diffuse intensities is closely similar to that applied to obtain the equations for the coherent amplitudes. For the total intensities, the following system of equations can be written:

$$\begin{cases} \dfrac{\partial I_0(q_{0_x}, z)}{\partial z} = \left\langle E_0^*(q_{0_x}, z) \dfrac{\partial E_0(q_{0_x}, z)}{\partial z} \right\rangle \\ \qquad + \left\langle \dfrac{\partial E_0^*(q_{0_x}, z)}{\partial z} E_0(q_{0_x}, z) \right\rangle \\ \dfrac{\partial I_h(q_{h_x}, z)}{\partial z} = \left\langle E_h^*(q_{h_x}, z) \dfrac{\partial E_h(q_{h_x}, z)}{\partial z} \right\rangle \\ \qquad + \left\langle \dfrac{\partial E_h^*(q_{h_x}, z)}{\partial z} E_h(q_{h_x}, z) \right\rangle . \end{cases} \quad (32)$$

We consider terms on the right-hand side of the system of equations (32) in detail.

$$\begin{aligned} &\left\langle E_0^*(q_{0_x}, z) \frac{\partial E_0(q_{0_x}, z)}{\partial z} \right\rangle \\ &\quad = i(a_0 - q_{0_x} \cot\theta_1) I_0(q_{0_x}, z) + \frac{i}{2\pi} \int \mathrm{d}x\, a_{\bar{h}} \exp(-iq_{0_x} x) \\ &\quad \times \int \mathrm{d}q_{h_x} \exp(iq_{h_x} x) \langle E_0^*(q_{0_x}, z) \exp[i\mathbf{h} \cdot \delta\mathbf{u}(x, z)] \\ &\quad \times E_h(q_{h_x}, z) \rangle \end{aligned} \quad (33)$$

$$\begin{aligned} &\left\langle E_h^*(q_{h_x}, z) \frac{\partial E_h(q_{h_x}, z)}{\partial z} \right\rangle \\ &\quad = -i(\eta' - a_0 - q_{h_x} \cot\theta_2) I_h(q_{h_x}, z) \\ &\quad - \frac{i}{2\pi} \int \mathrm{d}x\, a_h \exp(-iq_{h_x} x) \int \mathrm{d}q_{0_x} \exp(iq_{0_x} x) \\ &\quad \times \langle E_h^*(q_{h_x}, z) \exp[-i\mathbf{h} \cdot \delta\mathbf{u}(x, z)] E_0(q_{0_x}, z) \rangle . \end{aligned} \quad (34)$$

The correlation on the right-hand side of equation (33) can be given in the form

$$\langle E_0^* \Phi E_h \rangle = f \langle E_0^* E_h \rangle + \langle (E_0^* \delta\Phi) E_h \rangle + \langle E_0^* (\delta\Phi E_h) \rangle . \quad (35)$$

After substitution of the formal solutions (14*a*), (14*b*), we obtain for the last two terms on the right-hand side of equation (35):

$$\begin{aligned} \langle (E_0^* \delta\Phi) E_h \rangle &= \frac{i}{2\pi} a_h (1 - f^2) \int \mathrm{d}\tilde{q}_{0_x} \langle E_0^*(q_{0_x}, z) E_0(\tilde{q}_{0_x}, z) \rangle \\ &\quad \times \exp[-i(q_{h_x} - \tilde{q}_{0_x}) x] \hat{\tau}_1^c \end{aligned} \quad (36)$$

$$\begin{aligned} \langle E_0^* (\delta\Phi E_h) \rangle &= -\frac{i}{2\pi} a_{\bar{h}}^* (1 - f^2) \int \mathrm{d}\tilde{q}_{h_x} \langle E_h(q_{h_x}, z) E_h^*(\tilde{q}_{h_x}, z) \rangle \\ &\quad \times \exp[i(q_{0_x} - \tilde{q}_{h_x}) x] \hat{\tau}_2^{c*} . \end{aligned} \quad (37)$$

Similarly, we can transform the correlation $\langle E_h^* \Phi^* E_0 \rangle$ in equation (34).

Finally, we obtain the equations for the total intensities in the following form:

$$\begin{cases} \dfrac{\partial I_0(q_{0_x}, z)}{\partial z} = ia_0 I_0(q_{0_x}, z) + ia_{\bar{h}} f \langle E_0^*(q_{0_x}, z) E_h(q_{0_x}, z) \rangle \\ \qquad - a_h a_{\bar{h}} (1 - f^2) I_0(q_{0_x}, z) \bar{\tau}_1^c + \dfrac{1}{2\pi} |a_{\bar{h}}|^2 (1 - f^2) \\ \qquad \times \displaystyle\int \mathrm{d}q_{h_x} \langle E_h(q_{h_x}, z) E_h^*(q_{h_x}, z) \rangle \hat{\tau}_2^{c*} + \text{c.c.} \\ \dfrac{\partial I_h(q_{h_x}, z)}{\partial z} = -i(\eta' - a_0) I_h(q_{h_x}, z) \\ \qquad - ia_h f \langle E_h^*(q_{h_x}, z) E_0(q_{h_x}, z) \rangle \\ \qquad + a_h a_{\bar{h}} (1 - f^2) I_h(q_{h_x}, z) \bar{\tau}_2^c - \dfrac{1}{2\pi} |a_h|^2 (1 - f^2) \\ \qquad \times \displaystyle\int \mathrm{d}q_{0_x} \langle E_0(q_{0_x}, z) E_0^*(q_{0_x}, z) \rangle \hat{\tau}_1^{c*} + \text{c.c.} \end{cases} \quad (38)$$

By analogy with the procedure used for derivation of the equations for the total intensities, we develop the equations for the coherent intensities:

$$\begin{cases} \dfrac{\partial I_0^c(q_{0_x}, z)}{\partial z} = ia_0 I_0^c(q_{0_x}, z) + ia_{\bar{h}} f E_0^{c*}(q_{0_x}, z) E_h^c(q_{0_x}, z) \\ \qquad - a_h a_{\bar{h}} (1 - f^2) I_0^c(q_{0_x}, z) \bar{\tau}_1^c + \text{c.c.} \\ \dfrac{\partial I_h^c(q_{h_x}, z)}{\partial z} = i(a_0 - \eta') I_h^c(q_{h_x}, z) - ia_h f E_h^{c*}(q_{h_x}, z) E_0^c(q_{h_x}, z) \\ \qquad + a_h a_{\bar{h}} (1 - f^2) I_h^c(q_{h_x}, z) \bar{\tau}_2^c + \text{c.c.} \end{cases} \quad (39)$$

To obtain the equations for the diffuse intensities, the system of equations for the coherent intensities (39) should be subtracted from the system of equations for the total intensity (38). After some algebra, we obtain for the diffuse intensities:

$$\begin{aligned} \frac{\partial I_0^d(q_{0_x}, z)}{\partial z} &= ia_0 I_0^d(q_{0_x}, z) - a_h a_{\bar{h}} (1 - f^2) I_0^d(q_{0_x}, z) \bar{\tau}_1^c \\ &\quad - I_0^d(q_{0_x}, z) \int_z^l \mathrm{d}z'\, a_h a_{\bar{h}} f^2 \exp[i(z' - z)\eta'] \\ &\quad \times \langle \tilde{E}_0^{d*}(q_{0_x}, z) \tilde{E}_0^d(q_{0_x}, z') \rangle_0 \\ &\quad \times \exp\{-iq_{0_x}[(z' - z)\cot\theta_2]\} \\ &\quad + I_h^d(q_{0_x}, z) \int_0^z \mathrm{d}z' |a_{\bar{h}}|^2 f^2 \exp[i(z' - z)\eta'] \\ &\quad \times \langle \tilde{E}_h^d(q_{0_x}, z) \tilde{E}_h^{d*}(q_{0_x}, z') \rangle_H \\ &\quad \times \exp\{-iq_{0_x}[(z' - z)\cot\theta_2]\} \\ &\quad + \frac{1}{2\pi} |a_{\bar{h}}|^2 (1 - f^2) \int \mathrm{d}q_{h_x} I_h^c(q_{h_x}, z) \hat{\tau}_2^{c*} \\ &\quad + \frac{1}{2\pi} |a_{\bar{h}}|^2 (1 - f^2) \int \mathrm{d}q_{x_h} I_h^d(q_{h_x}, z) \hat{\tau}_2^{c*} + \text{c.c.} \end{aligned} \quad (40)$$

$$\frac{\partial I_h^d(q_{h_x},z)}{\partial z} = -i(\eta' - a_0)I_h^d(q_{h_x},z) + a_h a_{\bar{h}}(1-f^2)I_h^d(q_{h_x},z)\bar{\tau}_2^c$$
$$+ I_h^d(q_{h_x},z)\int_0^z \mathrm{d}z'\, a_h a_{\bar{h}} f^2 \exp[-i(z'-z)\eta']$$
$$\times \langle \tilde{E}_h^{d*}(q_{h_x},z)\tilde{E}_h^d(q_{h_x},z')\rangle_H$$
$$\times \exp\{iq_{h_x}[(z'-z)\cot\theta_2]\}$$
$$- I_0^d(q_{h_x},z)\int_z^l \mathrm{d}z'\, |a_h|^2 f^2 \exp[-i(z'-z)\eta'^*]$$
$$\times \langle \tilde{E}_0^d(q_{h_x},z)\tilde{E}_0^{d*}(q_{h_x},z')\rangle_0$$
$$\times \exp\{iq_{h_x}[(z'-z)\cot\theta_2]\}$$
$$- \frac{1}{2\pi}|a_h|^2(1-f^2)\int \mathrm{d}q_{0_x}\, I_0^c(q_{0_x},z)\hat{\tau}_1^{c*}$$
$$- \frac{1}{2\pi}|a_h|^2(1-f^2)\int \mathrm{d}q_{0_x}\, I_0^d(q_{0_x},z)\hat{\tau}_1^{c*} + \text{c.c.} \qquad (41)$$

Here, relations within $\langle\,\rangle_0$ and $\langle\,\rangle_H$ are normalized to the diffuse intensities I_0^d and I_h^d, respectively. Now we enter into consideration of the correlation lengths of the diffusely scattering waves:

$$\bar{\Gamma}_0(\eta', q_{0_x}, z) = \int_0^{l-z\approx\infty} \mathrm{d}\xi\, \exp[i\xi(\eta' - q_{0_x}\cot\theta_2)]$$
$$\times \langle \tilde{E}_0^{d*}(q_{0_x},z)\tilde{E}_0^d(q_{0_x},z+\xi)\rangle_0 \qquad (42)$$
$$\bar{\Gamma}_H(\eta', q_{0_x}, z) = \int_0^{z} \mathrm{d}\psi\, \exp[-i\psi(\eta' - q_{0_x}\cot\theta_2)]$$
$$\times \langle \tilde{E}_h^d(q_{0_x},z)\tilde{E}_h^{d*}(q_{0_x},z-\psi)\rangle_H. \qquad (43)$$

Finally, the equations for the diffuse intensities can be rewritten as

$$\frac{\partial I_0^d(q_{0_x},z)}{\partial z} = ia_0 I_0^d(q_{0_x},z) - a_h a_{\bar{h}}(1-f^2)I_0^d(q_{0_x},z)\bar{\tau}_1^c$$
$$- a_h a_{\bar{h}} f^2 I_0^d(q_{0_x},z)\bar{\Gamma}_0 + |a_{\bar{h}}|^2 f^2 I_h^d(q_{0_x},z)\bar{\Gamma}_H$$
$$+ \frac{1}{2\pi}|a_{\bar{h}}|^2(1-f^2)\int \mathrm{d}q_{h_x}\, I_h^d(q_{h_x},z)\hat{\tau}_2^{c*}$$
$$+ \frac{1}{2\pi}|a_{\bar{h}}|^2(1-f^2)\int \mathrm{d}q_{h_x}\, I_h^c(q_{h_x},z)\hat{\tau}_2^{c*} + \text{c.c.} \qquad (44)$$

$$\frac{\partial I_h^d(q_{h_x},z)}{\partial z} = -i(\eta' - a_0)I_h^d(q_{h_x},z) + a_h a_{\bar{h}}(1-f^2)I_h^d(q_{h_x},z)\bar{\tau}_2^c$$
$$+ a_h a_{\bar{h}} f^2 I_h^d(q_{h_x},z)\bar{\Gamma}_h^* - |a_h|^2 f^2 I_0^d(q_{h_x},z)\bar{\Gamma}_0^*$$
$$- \frac{1}{2\pi}|a_h|^2(1-f^2)\int \mathrm{d}q_{0_x}\, I_0^d(q_{0_x},z)\hat{\tau}_1^{c*}$$
$$- \frac{1}{2\pi}|a_h|^2(1-f^2)\int \mathrm{d}q_{0_x}\, I_0^c(q_{0_x},z)\hat{\tau}_1^{c*} + \text{c.c.} \qquad (45)$$

The first terms on the right-hand side of equations (44) and (45) describe the photoelectric absorption, the second ones determine the diffuse absorption, the third ones represent the attenuation as a result of diffraction of the diffuse waves, the fourth and the fifth ones are responsible for the diffraction of the diffuse waves, and the sixth ones define the sources of the diffuse waves inside the crystal.

In the case of kinematical diffraction, the system of equations for the coherent amplitudes (24) is simplified:

$$\begin{cases} \dfrac{\partial E_0^c(q_{0_x},z)}{\partial z} = i(a_0 - q_{0_x}\cot\theta_1)E_0^c(q_{0_x},z) \\ \dfrac{\partial E_h^c(q_{h_x},z)}{\partial z} = i(a_0 - \eta' + q_{h_x}\cot\theta_2)E_h^c(q_{h_x},z) \\ \qquad\qquad - ia_h f E_0^c(q_{h_x},z). \end{cases} \qquad (46)$$

Recently (Faleev *et al.*, 1999; Pavlov *et al.*, 1999), our approach in the semidynamical form was used for the determination of the principal parameters of vertically coupled InAs quantum dots (QDs) self-assembled in a GaAs matrix. The statistically disturbed QDs were described as kinds of structural defects and only the coherent intensity of the diffracted wave was taken into account.

For the diffuse intensities in the kinematical case, we obtain from (44) and (45):

$$\frac{\partial I_0^d(q_{0_x},z)}{\partial z} = ia_0 I_0^d(q_{0_x},z) + \text{c.c.} \qquad (47)$$
$$\frac{\partial I_h^d(q_{h_x},z)}{\partial z} = -i(\eta' - a_0)I_h^d(q_{h_x},z) - |a_h|^2 f^2 I_0^d(q_{h_x},z)\bar{\Gamma}_0^*$$
$$- \frac{1}{2\pi}|a_h|^2(1-f^2)\int \mathrm{d}q_{0_x}\, I_0^d(q_{0_x},z)\hat{\tau}_1^{c*}$$
$$- \frac{1}{2\pi}|a_h|^2(1-f^2)\int \mathrm{d}q_{0_x}\, I_0^c(q_{0_x},0)$$
$$\times \exp[-2\,\mathrm{Im}(a_0)z]\hat{\tau}_1^{c*} + \text{c.c.} \qquad (48)$$

In the ideal case, if a plane wave with intensity of unity falls on a crystal, there is only one Fourier component in the form of a delta function in the incident beam. And if the registration system works in the so-called θ–2θ mode ($q_h = 0$), then one can obtain from (24), (44) and (45) the equation for the plane-wave diffraction (Pavlov & Punegov, 1998*a*,*b*).

5. Concluding remarks

The new approach to Kato's variant of SDDT for simulating the intensity distribution in the reciprocal space is proposed in the case of statistically distributed microdefects. Compared to other approaches (Holý *et al.*, 1992, 1993, 1994; Darhuber *et al.*, 1997), our approach describes more correctly the scattering process in thick structures, where one has to take into account the dynamical interaction inside the wavefields.

APPENDIX *A*

For presentation, in the triple-crystal scheme we use a standard (+*n*, −*n*, +*n*) arrangement (Iida & Kohra, 1979; Zaumseil & Winter, 1982*a*,*b*). However, instead of θ and α (Iida & Kohra, 1979), for angular deviations we employ ε and ω, respectively. The differential variations of the scattering vector $\mathbf{q} = \mathbf{K}_H - \mathbf{K}_0$ near the Bragg reflection are given by (see Appendix in Herres *et al.*, 1996):

$$\delta q_z \approx -k[\cos(\theta_B + \varphi)\varepsilon + 2\sin(\theta_B)\sin(\varphi)\omega] \quad (49)$$

$$\delta q_x \approx -k[\sin(\theta_B + \varphi)\varepsilon - 2\sin(\theta_B)\cos(\varphi)\omega]. \quad (50)$$

These equations (49), (50) can be obtained from the simple geometrical construction for deviation vectors $\delta\mathbf{K}_0$ and $\delta\mathbf{K}_H$ (see Kazimirov *et al.*, 1990):

$$\delta K_{0z} = k\cos(\theta_B - \varphi)\omega, \quad \delta K_{0x} = -k\sin(\theta_B - \varphi)\omega, \quad (51)$$

$$\delta K_{Hz} = -k\cos(\theta_B + \varphi)(\varepsilon - \omega),$$
$$\delta K_{Hx} = -k\sin(\theta_B + \varphi)(\varepsilon - \omega), \quad (52)$$

since $\delta\mathbf{q} = \delta\mathbf{K}_H - \delta\mathbf{K}_0$. In the case of coherent scattering, the components δK_{0x} and δK_{Hx} should be the same if the crystal is homogeneous in the direction parallel to its surface. It results in $\varepsilon = \omega(1 + b)$ for coherent plane waves (so-called θ–2θ scan scheme) and transforms equations (49) and (50) as

$$\delta q_z \approx -k\omega\sin(2\theta_B)/\sin(\theta_B + \varphi) \quad (53)$$

$$\delta q_x = 0. \quad (54)$$

Here, in equation (53), δq_z is identical to the parameter $(-\eta')$ (9), exclusive of the term including the refraction effect.

In this paper, we take into consideration the pseudo-plane incident waves. This means that the position of the average wavevector of the incident wave determined by ω is not enough to describe the complex structure of the incident waves. Hence, we have to introduce the additional vector $\mathbf{q}_0$, which describes the deviation of the Fourier-component wavevector from the average wavevector $\mathbf{K}_0$ of the incident wave. By analogy, we may assume that

$$q_{0z} = k\cos(\theta_B - \varphi)\omega', \quad q_{0x} = -k\sin(\theta_B - \varphi)\omega', \quad (55)$$

where ω' describes the deviation of the wavevector of any Fourier component of the incident wavefield from the average wavevector $\mathbf{K}_0$. In the case of an ideal plane wave, there is only one nonzero Fourier component with $\omega' = 0$. The components of the vector $\mathbf{q}_H$ are given by

$$q_{Hz} = -k\cos(\theta_B + \varphi)[\varepsilon - \omega(1 + b)],$$
$$q_{Hx} = -k\sin(\theta_B + \varphi)[\varepsilon - \omega(1 + b)]. \quad (56)$$

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