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# The Equations of the Statistical Dynamical Theory of X-ray Diffraction for Deformed Crystals

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## Abstract

Using the statistical approach to dynamical X-ray diffraction, the equations for coherent and diffuse scattered waves in a general case of a deformed crystal are obtained.

## 1. Introduction

The statistical dynamical theory of a diffraction for a point source in Laue geometry was first developed by Kato (1980). This theory was modernized by Bushuev (1989*a*,*b*) taking the angular distribution of coherently and diffusely scattered waves into account. Earlier, this problem was considered by Holý (1982*a*,*b*) on the basis of the introduction of mutual coherence functions. The statistical dynamical theories of diffraction in one-dimensionally deformed crystals (Punegov, 1990*a*,*b*; Punegov, Petrakov & Tikhonov, 1990; Punegov & Vishnjakov, 1995) and multilayer systems (Punegov, 1991, 1992, 1993) were used for interpretation of some experimental results (Pavlov *et al.*, 1995; Li *et al.*, 1995). The aim of this work is to develop the statistical dynamical theory of X-ray diffraction for a general case of a deformed crystal.

We consider Bragg diffraction from a deformed crystal containing statistically distributed microdefects. In the so-called coherent approximation, the X-ray diffraction on a deformed crystal without statistically distributed defects is described by well known differential equations (Takagi, 1969; Taupin, 1964). As distinct from Kato's (1980) theory, we take the angular distribution of scattered intensities (case of plane waves) and also the variation of interplanar spacing into account. In our consideration, it is convenient to use the system of differential equations for amplitudes of the transmitted $E_0$ and diffracted $E_h$ waves in the form [see equation (2.23) in Afanas'ev & Kohn, 1971]:

$$\begin{aligned}\partial E_0/\partial s_0 &= (i\pi/\lambda)E_0\chi_0 + (i\pi/\lambda)\chi_{\bar h}C\exp(i\mathbf{h}\cdot\mathbf{u})E_h\\ \partial E_h/\partial s_h &= (i\pi/\lambda)E_h(\chi_0-\alpha_h)\\ &\quad + (i\pi/\lambda)\chi_h C\exp(-i\mathbf{h}\cdot\mathbf{u})E_0,\end{aligned} \qquad (1)$$

where $\mathbf{h}$ is the vector of diffraction, $\chi_{0,h,\bar h}$ are the Fourier components of the susceptibility, $\lambda$ is the X-ray wavelength and $\kappa = 2\pi/\lambda$. The total displacement of atoms from their positions in a perfect lattice can be written as $\mathbf{u} = \langle\mathbf{u}\rangle + \delta\mathbf{u}$, where $\delta\mathbf{u}$ is the fluctuational displacement caused by microdefects, $\langle\mathbf{u}\rangle$ is the average atomic displacement,

$$C = \begin{cases} 1 & \text{for } \sigma \text{ polarization} \\ \cos(2\theta_0) & \text{for } \pi \text{ polarization,} \end{cases}$$

$\alpha_h = -2\sin 2\theta_0\omega$ and $\omega = \theta - \theta_0$ is the deviation from Bragg angle $\theta_0$.

## 2. Theory

Let a monochromatic X-ray plane wave fall on a deformed crystal containing statistically distributed microdefects. We shall direct the axes $s_0$ and $s_h$ of an oblique-angled system of coordinates on the wavevector $\mathbf{k}_0$ of the transmitted wave and on the wavevector $\mathbf{k}_h$ of the diffracted wave. For a Cartesian system of coordinates, the axis $Z$ is directed into the crystal and the axis $X$ is directed along the surface of the crystal (see Fig. 1). The axis $Y$ is directed along the surface of the crystal and is perpendicular to axes $X$ and $Z$.

The relationship between the oblique-angled coordinate system $(s_0, s_h)$ and the Cartesian system $(X, Z)$ is given by

$$\begin{aligned} s_0 &\approx [\sin(2\theta_0)]^{-1}[x\sin(\theta_0+\varphi) + z\cos(\theta_0+\varphi)]\\ s_h &\approx [\sin(2\theta_0)]^{-1}[x\sin(\theta_0-\varphi) - z\cos(\theta_0-\varphi)]\\ x &= s_0\cos(\theta_0-\varphi) + s_h\cos(\theta_0+\varphi)\\ z &= s_0\sin(\theta_0-\varphi) - s_h\sin(\theta_0+\varphi),\end{aligned} \qquad (2)$$

where $\varphi$ is the inclination of the lattice planes with the crystal surface. The boundary conditions for Bragg geometry are defined as follows:

$$\begin{aligned} E_0[z=0 \Leftrightarrow (\hat s_0, \hat s_h)] &= E_0^{(\mathrm{in})}(x,0),\\ E_h[z=l \Leftrightarrow (\bar s_0, \bar s_h)] &= 0. \end{aligned} \qquad (3)$$

Here, $E_0^{(\mathrm{in})}(x,0)$ is the amplitude of the X-ray incident wave of the entrance surface. For simplification of the further theoretical calculations, we take $E_0^{(\mathrm{in})}(x,0) = 1$.

We make the following transformations in expressions for the amplitude of incident and transmitted waves:

$$\tilde{E}_0(s_0, s_h) = E_0(s_0, s_h)\exp[-(i\pi/\lambda)\chi_0(s_0 - s_h/b)]$$
$$\tilde{E}_h(s_0, s_h) = E_h(s_0, s_h)\exp[-(i\pi/\lambda)(\chi_0 - \alpha_h)(s_h - s_0 b)], \quad (4)$$

where $b = \sin(\theta_1)/\sin(\theta_2) = \sin(\theta_0 - \varphi)/\sin(\theta_0 + \varphi)$ is the asymmetry factor.

The set of Takagi equations (1) may be rewritten as

$$\begin{aligned} &\partial\tilde{E}_0(s_0, s_h)/\partial s_0 \\ &\quad = (i\pi/\lambda)\chi_{\bar{h}} C\exp(i\mathbf{h}\cdot\mathbf{u})\tilde{E}_h(s_0, s_h) \\ &\qquad \times \exp\{(i\pi/\lambda)[(s_h/b) - s_0][\chi_0(1+b) - b\alpha_h]\} \\ &\partial\tilde{E}_h(s_0, s_h)/\partial s_h \\ &\quad = (i\pi/\lambda)\chi_h C\exp(-i\mathbf{h}\cdot\mathbf{u})\tilde{E}_0(s_0, s_h) \\ &\qquad \times \exp\{(i\pi/\lambda)(s_0 - s_h/b)[\chi_0(1+b) - b\alpha_h]\}. \end{aligned} \quad (5)$$

It is possible to write the formal solution of the set of the differential equations (5) as

$$\begin{aligned} \tilde{E}_0(s_0, s_h) = {} & \tilde{E}_0(\hat{s}_0, \hat{s}_h) + \int_{\hat{s}_0(\text{along } s_h)}^{s_0} ds'_0\,(i\pi/\lambda)\chi_{\bar{h}} C \\ & \times \exp[i\mathbf{h}\cdot\mathbf{u}(s'_0, s_h)]\exp\{(i\pi/\lambda)(s_h/b - s'_0) \\ & \times [\chi_0(1+b) - b\alpha_h]\}\tilde{E}_h(s'_0, s_h) \end{aligned} \quad (6)$$

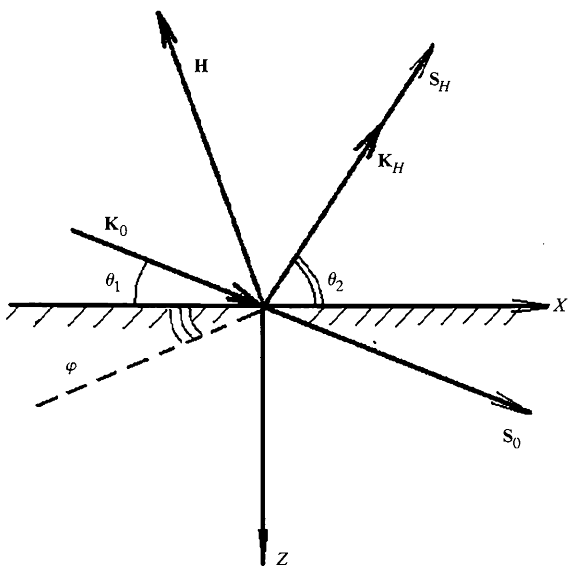


Fig. 1. Scheme of diffraction. $\mathbf{K}_0$ is the wavevector of the transmitted wave, $\mathbf{K}_H$ is the wavevector of the diffracted wave, $\mathbf{H}$ is the diffraction vector and $\varphi$ is the inclination of the lattice planes with the crystal.

$$\begin{aligned} \tilde{E}_h(s_0, s_h) = {} & \tilde{E}_h(\bar{s}_0, \bar{s}_h) + \int_{\bar{s}_h(\text{along } s_0)}^{s_h} ds'_h\,(i\pi/\lambda)\chi_h C \\ & \times \exp[-i\mathbf{h}\cdot\mathbf{u}(s_0, s'_h)]\exp\{(i\pi/\lambda) \\ & \times (s_0 - s'_h/b)[\chi_0(1+b) - b\alpha_h]\}\tilde{E}_0(s_0, s'_h). \end{aligned} \quad (7)$$

We execute a statistical average of set (5) and take into account

$$\begin{aligned} \exp[i\mathbf{h}\cdot\mathbf{u}(s_0, s_h)] &= \exp(i\mathbf{h}\langle\mathbf{u}\rangle)\exp(i\mathbf{h}\cdot\delta\mathbf{u}) \\ &= \exp(i\mathbf{h}\langle\mathbf{u}\rangle)\Phi \\ &= \exp[i\mathbf{h}\langle\mathbf{u}\rangle](\langle\Phi\rangle + \delta\Phi) \\ &= \exp[i\mathbf{h}\langle\mathbf{u}(s_0, s_h)\rangle] \\ &\quad \times [E(s_0, s_h) + \delta\Phi(s_0, s_h)]. \end{aligned} \quad (8)$$

Here, $E = E(s_0, s_h)$ is the static Debye–Waller factor. In our theory, this factor characterizes the distortions of a crystal lattice caused by statistically distributed defects. In a general case, lattice defects are non-uniformly distributed on a crystal volume. Therefore, in our theory, the static Debye–Waller factor depends on two coordinates. A statistical average is taken along an axis $Y$. In experiments, this corresponds to integration by the detector of scattered intensity along an axis $Y$. Such an average differs from corresponding ones of previous works.

In Kato's (1980) theory, the average is taken on a crystal volume. Therefore, the static factor does not depend on coordinates. In other works (Punegov, 1991; Holý *et al.*, 1992), the layer-by-layer average (parallel to the surface of a crystal) enables one to obtain the static Debye–Waller factor depending only on one coordinate $Z$.

The amplitudes of coherent waves $\tilde{E}^c_{0,h} = \langle\tilde{E}_{0,h}\rangle$ are slowly varying functions in comparison with the fluctuation of the lattice phase factor $\delta\Phi$. Hence, the correlation between $\tilde{E}^c_{0,h}$ and $\delta\Phi$ can be neglected. We obtain the following system of equations:

$$\begin{aligned} &\partial\tilde{E}^c_0(s_0, s_h)/\partial s_0 \\ &\quad = (i\pi/\lambda)\chi_{\bar{h}} C\exp\{(i\pi/\lambda)(s_h/b - s_0) \\ &\qquad \times [\chi_0(1+b) - b\alpha_h]\}\exp[i\mathbf{h}\langle\mathbf{u}(s_0, s_h)\rangle] \\ &\qquad \times \Bigg[E(s_0, s_h)\tilde{E}^c_h(s_0, s_h) \\ &\qquad + \int_{\bar{s}_h(\text{along } s_0)}^{s_h} (ds'_h\,(i\pi/\lambda)\chi_h C\langle\delta\Phi(s_0, s_h)\delta\Phi^*(s_0, s'_h)\rangle \\ &\qquad \times \exp\{(i\pi/\lambda)(s_0 - s'_h/b)[\chi_0(1+b) - b\alpha_h]\} \\ &\qquad \times \exp\{i\mathbf{h}[-\langle\mathbf{u}(s_0, s'_h)\rangle]\}\tilde{E}^c_0(s_0, s'_h))\Bigg] \end{aligned}$$

$$\begin{aligned}
&\partial \tilde{E}_h^c(s_0, s_h)/\partial s_h \\
&\quad = (i\pi/\lambda)\chi_h C \exp\{(i\pi/\lambda)(s_0 - s_h/b) \\
&\qquad \times [\chi_0(1+b) - b\alpha_h]\} \exp[-i\mathbf{h}\langle \mathbf{u}(s_0, s_h)\rangle] \\
&\qquad \times \Bigg[ E(s_0, s_h)\tilde{E}_0^c(s_0, s_h) \\
&\qquad + \int_{\tilde{s}_0(\text{along } s_h)}^{s_0} \Big(ds_0'\,(i\pi/\lambda)\chi_{\bar h} C\langle \delta\Phi^*(s_0, s_h)\delta\Phi(s_0', s_h)\rangle \\
&\qquad \times \exp\{(i\pi/\lambda)(s_h/b - s_0')[\chi_0(1+b) - b\alpha_h]\} \\
&\qquad \times \exp\{-i\mathbf{h}[-\langle \mathbf{u}(s_0', s_h)\rangle]\}\tilde{E}_h^c(s_0', s_h)\Big)\Bigg].
\end{aligned} \tag{9}$$

The coherent amplitudes $\tilde{E}_{0,h}^c$ slowly change with length $\tau_0 \ll \Lambda$, where $\tau_0$ is Kato's correlation length (Kato, 1980), $\Lambda = \Lambda_{\text{perf}}/E$ is the extinction length of a crystal with defects and $\Lambda_{\text{perf}}$ is the extinction length of a perfect crystal. The amplitude of coherently scattered waves $\tilde{E}_{0,h}^c$ can be taken from under the integrals in (9).

We return to a set for initial amplitudes:

$$\begin{aligned}
&\partial E_0^c(s_0, s_h)/\partial s_0 \\
&\quad = (i\pi/\lambda)\chi_0 E_0^c(s_0, s_h) + (i\pi/\lambda)\chi_{\bar h} C E(s_0, s_h) \\
&\qquad \times E_h^c(s_0, s_h) \exp[i\mathbf{h}\langle \mathbf{u}(s_0, s_h)\rangle] \\
&\qquad - (\pi^2/\lambda^2)\chi_h\chi_{\bar h} C^2 E_0^c(s_0, s_h) \\
&\qquad \times \int_{\tilde{s}_h(\text{along } s_0)}^{s_h} \Big(ds_h'\,\langle \delta\Phi(s_0, s_h)\delta\Phi^*(s_0, s_h')\rangle \\
&\qquad \times \exp\{i\mathbf{h}[\langle \mathbf{u}(s_0, s_h)\rangle - \langle \mathbf{u}(s_0, s_h')\rangle]\} \\
&\qquad \times \exp\{(i\pi/\lambda)[(s_h - s_h')/b][\chi_0(1+b) - b\alpha_h]\}\Big) \\
&\partial E_h^c(s_0, s_h)/\partial s_h \\
&\quad = (i\pi/\lambda)(\chi_0 - \alpha_h)E_h^c(s_0, s_h) + (i\pi/\lambda)\chi_h C E(s_0, s_h) \\
&\qquad \times E_0^c(s_0, s_h) \exp[-i\mathbf{h}\langle \mathbf{u}(s_0, s_h)\rangle] \\
&\qquad - (\pi^2/\lambda^2)\chi_{\bar h}\chi_h C^2 E_h^c(s_0, s_h) \\
&\qquad \times \int_{\tilde{s}_0(\text{along } s_h)}^{s_0} \Big(ds_0'\,\langle \delta\Phi^*(s_0, s_h)\delta\Phi(s_0', s_h)\rangle \\
&\qquad \times \exp\{-i\mathbf{h}[\langle \mathbf{u}(s_0, s_h)\rangle - \langle \mathbf{u}(s_0', s_h)\rangle]\} \\
&\qquad \times \exp\{(i\pi/\lambda)(s_0 - s_0')[\chi_0(1+b) - b\alpha_h]\}\Big).
\end{aligned} \tag{10}$$

We introduce the correlation lengths

$$\begin{aligned}
\tau_1^c(s_0, s_h, \eta') = &\int_{0(\text{along } s_0)}^{s_h - \tilde{s}_h \approx \infty} d\xi\,\{\langle \delta\Phi(s_0, s_h)\delta\Phi^*(s_0, s_h - \xi)\rangle \\
&\times [1 - E(s_0, s_h)^2]^{-1}\} \exp\{i\mathbf{h}[\langle \mathbf{u}(s_0, s_h)\rangle \\
&- \langle \mathbf{u}(s_0, s_h - \xi)\rangle]\} \exp(i\xi\eta' \sin\theta_2)
\end{aligned} \tag{11}$$

$$\begin{aligned}
\tau_2^c(s_0, s_h, \eta') = &\int_{0(\text{along } s_h)}^{s_0 - \tilde{s}_0 \approx \infty} d\psi\,\{\langle \delta\Phi^*(s_0, s_h)\delta\Phi(s_0 - \psi, s_h)\rangle \\
&\times [1 - E(s_0, s_h)^2]^{-1}\} \exp\{-i\mathbf{h}[\langle \mathbf{u}(s_0, s_h)\rangle \\
&- \langle \mathbf{u}(s_0 - \psi, s_h)\rangle]\} \exp(i\psi\eta' \sin\theta_1).
\end{aligned} \tag{12}$$

These correlation lengths are functions of angular parameter $\eta' = (\kappa/2\sin\theta_1)[\chi_0(1+b) - b\alpha_h]$ and coordinates $s_0, s_h$. In a Cartesian system of coordinates, the correlation lengths can be written

$$\begin{aligned}
\tau_1^c(x, z, \eta') = &\int_0^{l - z \approx \infty} d\xi\,(1/\sin\theta_2) \\
&\times \{\langle \delta\Phi(x, z)\delta\Phi^*(x - \xi\cot\theta_2, z + \xi)\rangle \\
&\times [1 - E(x, z)^2]^{-1}\} \exp\{i\mathbf{h}[\langle \mathbf{u}(x, z)\rangle \\
&- \langle \mathbf{u}(x - \xi\cot\theta_2, z + \xi)\rangle]\} \exp(i\xi\eta')
\end{aligned} \tag{13}$$

$$\begin{aligned}
\tau_2^c(x, z, \eta') = &\int_0^{z \approx \infty} d\psi\,(1/\sin\theta_1) \\
&\times \{\langle \delta\Phi^*(x, z)\delta\Phi(x + \psi\cot\theta_1, z + \psi)\rangle \\
&\times [1 - E(x, z)^2]^{-1}\} \exp\{-i\mathbf{h}[\langle \mathbf{u}(x, z)\rangle \\
&- \langle \mathbf{u}(x + \psi\cot\theta_1, z + \psi)\rangle]\} \exp(-i\psi\eta').
\end{aligned} \tag{14}$$

The correlation lengths (13) and (14) differ in their integration directions. For $\tau_1^c(x, z, \eta')$, the integration is taken in the direction of a diffracted wave but, for $\tau_2^c(x, z, \eta')$, the integration is taken in the direction of a transmitted wave. The correlation lengths (13) and (14) include the correlation functions

$$g_1(x, z, \xi) = \langle \delta\Phi(x, z)\delta\Phi^*(x - \xi\cot\theta_2, z + \xi)\rangle \tag{15}$$

$$g_2(x, z, \xi) = \langle \delta\Phi^*(x, z)\delta\Phi(x + \psi\cot\theta_1, z + \psi)\rangle. \tag{16}$$

In a general case, the correlation functions $g_1$ and $g_2$ differ owing to non-uniform distribution of defects in a crystal. If the defect distribution is uniform and the average strain field $\langle \mathbf{u}\rangle = 0$ (when angular parameter $\eta' = 0$), the correlation lengths (11)–(14) transform into Kato's correlation length $\tau_0$. Then the set of equations (10) for coherent amplitudes is given by

$$\begin{aligned}
\partial E_0^c(s_0, s_h)/\partial s_0 = &(i\pi/\lambda)\chi_0 E_0^c(s_0, s_h) + (i\pi/\lambda)\chi_{\bar h} C \\
&\times E(s_0, s_h) \exp[i\mathbf{h}\langle \mathbf{u}(s_0, s_h)\rangle] E_h^c(s_0, s_h) \\
&- (\pi^2/\lambda^2)\chi_h\chi_{\bar h} C^2 E_0^c(s_0, s_h) \\
&\times \tau_1^c(s_0, s_h, \eta')[1 - E(s_0, s_h)^2] \\
\partial E_h^c(s_0, s_h)/\partial s_h = &(i\pi/\lambda)(\chi_0 - \alpha_h)E_h^c(s_0, s_h) + (i\pi/\lambda)\chi_h \\
&\times C E(s_0, s_h) \exp[-i\mathbf{h}\langle \mathbf{u}(s_0, s_h)\rangle] \\
&\times E_0^c(s_0, s_h) - (\pi^2/\lambda^2)\chi_{\bar h}\chi_h C^2 \\
&\times E_h^c(s_0, s_h)\tau_2^c(s_0, s_h, \eta')[1 - E(s_0, s_h)^2].
\end{aligned} \tag{17}$$

If there is no dependence on coordinate $x$, the set of equations (17) describes the X-ray diffraction from one-dimensionally distorted crystals (Punegov *et al.*, 1990).

The diffusely scattered intensity is equal to the difference between the total scattered intensity and the coherently scattered intensity:

$$I^d_{0,h} = \langle E_{0,h}E^*_{0,h}\rangle - \langle E_{0,h}\rangle\langle E^*_{0,h}\rangle. \quad (18)$$

Using the well known theoretical calculation of the statistical dynamical diffraction theory (Kato, 1980; Bushuev, 1989*a*,*b*), we obtain a set of equations for diffusely scattered intensities. For total scattered intensities, the system of equations can be written

$$\begin{aligned} \partial I_0(s_0,s_h)/\partial s_0 &= \langle E^*_0(s_0,s_h)[\partial E_0(s_0,s_h)/\partial s_0]\rangle \\ &\quad + \langle[\partial E^*_0(s_0,s_h)/\partial s_0]E_0(s_0,s_h)\rangle \\ \partial I_h(s_0,s_h)/\partial s_h &= \langle E^*_h(s_0,s_h)[\partial E_h(s_0,s_h)/\partial s_h]\rangle \\ &\quad + \langle[\partial E^*_h(s_0,s_h)/\partial s_h]E_h(s_0,s_h)\rangle. \end{aligned} \quad (19)$$

We consider in detail the first term on the right-hand side of the first equation of (19):

$$\begin{aligned} &\langle E^*_0(s_0,s_h)[\partial E_0(s_0,s_h)/\partial s_0]\rangle \\ &\quad = \Big\langle E^*_0(s_0,s_h)\{(i\pi/\lambda)E_0(s_0,s_h)\chi_0 \\ &\qquad + (i\pi/\lambda)\chi_{\bar h}C\Phi(s_0,s_h)\exp[i\mathbf{h}\langle\mathbf{u}(s_0,s_h)\rangle]E_h(s_0,s_h)\}\Big\rangle \\ &\quad = (i\pi/\lambda)\chi_0 I_0(s_0,s_h) + (i\pi/\lambda)\chi_{\bar h}C \\ &\qquad \times\langle E^*_0(s_0,s_h)\Phi(s_0,s_h)E_h(s_0,s_h)\rangle\exp[i\mathbf{h}\langle\mathbf{u}(s_0,s_h)\rangle]. \end{aligned} \quad (20)$$

We convert the second term in the right part of (20):

$$\begin{aligned} &\langle E^*_0(s_0,s_h)\Phi(s_0,s_h)E_h(s_0,s_h)\rangle\exp[i\mathbf{h}\langle\mathbf{u}(s_0,s_h)\rangle] \\ &\quad = E(s_0,s_h)\langle E^*_0(s_0,s_h)E_h(s_0,s_h)\rangle\exp[i\mathbf{h}\langle\mathbf{u}(s_0,s_h)\rangle] \\ &\qquad + \langle[E^*_0(s_0,s_h)\delta\Phi(s_0,s_h)]E_h(s_0,s_h)\rangle\exp[i\mathbf{h}\langle\mathbf{u}(s_0,s_h)\rangle] \\ &\qquad + \langle E^*_0(s_0,s_h)[\delta\Phi(s_0,s_h)E_h(s_0,s_h)]\rangle\exp[i\mathbf{h}\langle\mathbf{u}(s_0,s_h)\rangle] \\ &\quad = E(s_0,s_h)\langle E^*_0(s_0,s_h)E_h(s_0,s_h)\rangle\exp[i\mathbf{h}\langle\mathbf{u}(s_0,s_h)\rangle] \\ &\qquad + \Big\langle[E^*_0(s_0,s_h)\delta\Phi(s_0,s_h)]\exp[i\mathbf{h}\langle\mathbf{u}(s_0,s_h)\rangle] \\ &\qquad \times\int\limits_{\bar s_h(\text{along } s_0)}^{s_h} ds'_h\,(i\pi/\lambda)\chi_h C\exp[-i\mathbf{h}\cdot\mathbf{u}(s_0,s'_h)] \\ &\qquad \times\exp\big((i\pi/\lambda)\{[(s_h-s'_h)/b][\chi_0(1+b)-b\alpha_h]\}\big) \\ &\qquad \times E_0(s_0,s'_h)\Big\rangle + \Big\langle[\delta\Phi(s_0,s_h)E_h(s_0,s_h)] \\ &\qquad \times\exp[i\mathbf{h}\langle\mathbf{u}(s_0,s_h)\rangle]\Big[-\int\limits_{\hat s_0(\text{along } s_h)}^{s_0} ds'_0\,(i\pi/\lambda)\chi^*_{\bar h}C \\ &\qquad \times\exp[-i\mathbf{h}\cdot\mathbf{u}(s'_0,s_h)]\exp\big(-(i\pi/\lambda)\{(s_0-s'_0) \\ &\qquad \times[\chi^*_0(1+b)-b\alpha_h]\}\big)E^*_h(s'_0,s_h)\Big]\Big\rangle. \end{aligned} \quad (21)$$

Similar consideration of other terms in (19) allows the system of equations for total scattered intensities to be obtained:

$$\begin{aligned} \partial I_0/\partial s_0 &= (i\pi/\lambda)\chi_0 I_0 + (i\pi/\lambda)\chi_{\bar h}CE\langle E^*_0E_h\rangle\exp(i\mathbf{h}\langle\mathbf{u}\rangle) \\ &\quad - (\pi^2/\lambda^2)\chi_h\chi_{\bar h}C^2I_0(1-E^2)\tau^c_1 \\ &\quad + (\pi^2/\lambda^2)|\chi_{\bar h}|^2C^2I_h(1-E^2)\tau^{c*}_2 + \text{c.c.} \\ \partial I_h/\partial s_h &= (i\pi/\lambda)(\chi_0-\alpha_h)I_h + (i\pi/\lambda)\chi_hCE\langle E^*_hE_0\rangle \\ &\quad \times\exp(-i\mathbf{h}\langle\mathbf{u}\rangle) - (\pi^2/\lambda^2)\chi_h\chi_{\bar h}C^2I_h(1-E^2)\tau^c_2 \\ &\quad + (\pi^2/\lambda^2)|\chi_h|^2C^2I_0(1-E^2)\tau^{c*}_1 + \text{c.c.} \end{aligned} \quad (22)$$

In (22) and the following expressions, we do not write down the arguments of the corresponding functions. For coherent scattered intensities, we find the following system of equations:

$$\begin{aligned} \partial I^c_0/\partial s_0 &= (i\pi/\lambda)\chi_0I^c_0 + (i\pi/\lambda)\chi_{\bar h}CE\exp(i\mathbf{h}\langle\mathbf{u}\rangle)E^{c*}_0E^c_h \\ &\quad - (\pi^2/\lambda^2)\chi_h\chi_{\bar h}C^2I^c_0\tau^c_1(1-E^2) + \text{c.c.} \\ \partial I^c_h/\partial s_h &= (i\pi/\lambda)(\chi_0-\alpha_h)I^c_h + (i\pi/\lambda)\chi_hCE \\ &\quad \times\exp(-i\mathbf{h}\langle\mathbf{u}\rangle)E^{c*}_hE^c_0 \\ &\quad - (\pi^2/\lambda^2)\chi_{\bar h}\chi_hC^2I^c_h\tau^c_2(1-E^2) + \text{c.c.} \end{aligned} \quad (23)$$

From (22) and (23), we obtain the system of equations for diffusely scattered intensities:

$$\begin{aligned} \partial I^d_0(s_0,s_h)/\partial s_0 &= \{-2\,\text{Im}[(\pi/\lambda)\chi_0] \\ &\quad - 2\,\text{Re}[(\pi^2/\lambda^2)\chi_h\chi_{\bar h}C^2(1-E^2)\tau^c_1] \\ &\quad - 2\,\text{Re}[(\pi^2/\lambda^2)\chi_h\chi_{\bar h}C^2E^2\Gamma_0]\}I^d_0 \\ &\quad + \{2(\pi^2/\lambda^2)|\chi_{\bar h}|^2C^2(1-E^2)\,\text{Re}(\tau^c_2) \\ &\quad + 2(\pi^2/\lambda^2)|\chi_{\bar h}|^2C^2E^2\,\text{Re}(\Gamma_H)\}I^d_h \\ &\quad + 2(\pi^2/\lambda^2)|\chi_{\bar h}|^2C^2(1-E^2)\,\text{Re}(\tau^c_2)I^c_h \\ \partial I^d_h(s_0,s_h)/\partial s_h &= \{-2\,\text{Im}[(\pi/\lambda)(\chi_0-\alpha_h)] \\ &\quad - 2\,\text{Re}[(\pi^2/\lambda^2)\chi_h\chi_{\bar h}C^2(1-E^2)\tau^c_2] \\ &\quad - 2\,\text{Re}[(\pi^2/\lambda^2)\chi_h\chi_{\bar h}C^2E^2\Gamma_h]\}I^d_h \\ &\quad + \{2(\pi^2/\lambda^2)|\chi_h|^2C^2(1-E^2)\,\text{Re}(\tau^c_1) \\ &\quad + 2(\pi^2/\lambda^2)|\chi_h|^2C^2E^2\,\text{Re}(\Gamma_0)\}I^d_0 \\ &\quad + 2(\pi^2/\lambda^2)|\chi_h|^2C^2(1-E^2)\,\text{Re}(\tau^c_1)I^c_0, \end{aligned} \quad (24)$$

where the correlation lengths

$$\begin{aligned} \Gamma_0(s_0,s_h,\eta') &= \int\limits_{0(\text{along } s_0)}^{s_h-\bar s_h\approx\infty} d\xi\,\langle\delta E^*_0(s_0,s_h)\delta E_0(s_0,s_h-\xi)\rangle_0 \\ &\quad \times\exp\{i\mathbf{h}[\langle\mathbf{u}(s_0,s_h)\rangle - \langle\mathbf{u}(s_0,s_h-\xi)\rangle]\} \\ &\quad \times\exp(i\eta'\xi\sin\theta_2) \\ \Gamma_h(s_0,s_h,\eta') &= \int\limits_{0(\text{along } s_h)}^{s_0-\hat s_0\approx\infty} d\psi\,\langle\delta E^*_h(s_0,s_h)\delta E_h(s_0-\psi,s_h)\rangle_h \\ &\quad \times\exp\{-i\mathbf{h}[\langle\mathbf{u}(s_0,s_h)\rangle - \langle\mathbf{u}(s_0-\psi,s_h)\rangle]\} \\ &\quad \times\exp(i\eta'\psi\sin\theta_1) \end{aligned} \quad (25)$$

are responsible for coherent scattering of incoherent waves on an 'average' lattice. Here, the fluctuation waves $\delta E_0(s_0, s_h)$ and $\delta E_h(s_0, s_h)$ are normalized to the appropriate diffuse intensities.

The analysis of correlation lengths $\Gamma_{0,h}$ is a separate problem. This problem is considered in detail by Bushuev (1994). It is shown that integrated $\Gamma_0$ can be written as

$$\Gamma_0 = c\tau_0(E\tau_0/\Lambda_{\rm perf}) \ll \tau_0, \Lambda_{\rm perf}. \qquad (26)$$

The coefficient $c$ ($c \approx 1$) depends on kinds of functions $\tau^c_{1,2}$ and $\Gamma_{0,h}$. For representation (26), the limiting transition can be taken as $E^2\Gamma_0 \to 0$ when $\tau_0 \to 0$ and $E \to 0$. Relation (26) also shows that the efficiency of dynamical diffuse scattering increases in a more perfect crystal.

In the kinematical limit, the equation for diffuse intensities is much simplified:

$$\begin{aligned}\partial I^d_0(s_0, s_h)/\partial s_0 &= \{-2\,{\rm Im}[(\pi/\lambda)\chi_0]\}I^d_0\\ \partial I^d_h(s_0, s_h)/\partial s_h &= \{-2\,{\rm Im}[(\pi/\lambda)(\chi_0 - \alpha_h)]\}I^d_h\\ &\quad + 2(\pi^2/\lambda^2)|\chi_h|^2C^2(1-E^2)\,{\rm Re}(\tau^c_1)I^c_0.\end{aligned} \qquad (27)$$

The set of equations for diffuse intensities (24) together with the system of the equations for coherent amplitudes (17) completely describe dynamical diffraction of X-ray beams by deformed crystals with statistically distributed defects.

In the case of kinematical X-ray diffraction, the formal solution for diffracted waves can be given in the form

$$\begin{aligned}E_h(s_0, s_h) &= \exp[(i\pi/\lambda)\chi_0 s_0]\exp[(i\pi/\lambda)(\chi_0 - \alpha_h)s_h]\\ &\quad\times \int_{\bar{s}_h(\text{along } s_0)}^{s_h} (i\pi/\lambda)\chi_h C\exp[-i\mathbf{h}\cdot\mathbf{u}(s_0, s'_h)]\\ &\quad\times \exp(-i\eta' s'_h \sin\theta_2)\,{\rm d}s'_h.\end{aligned} \qquad (28)$$

In a Cartesian system of coordinates, the solution (28) can be rewritten as

$$\begin{aligned}E_h(x, z) &= \exp[-(i\pi/\lambda)(\chi_0 - \alpha_h)(z/\sin\theta_2)]\int_z^l (i\pi/\lambda)\\ &\quad\times \chi_h C\exp\{-i\mathbf{h}\cdot\mathbf{u}[x-(z'-z)\cot\theta_2, z']\}\\ &\quad\times \exp(+i\eta' z')\,{\rm d}z'/\sin\theta_2.\end{aligned} \qquad (29)$$

For coherent amplitudes, we obtain

$$\begin{aligned}E^c_h(s_0, s_h) &= \exp\{(i\pi/\lambda)[\chi_0 s_0 + (\chi_0 - \alpha_h)s_h]\}\\ &\quad\times \int_{\bar{s}_h(\text{along } s_0)}^{s_h} (i\pi/\lambda)\chi_h C\exp[-i\mathbf{h}\langle\mathbf{u}(s_0, s'_h)\rangle]\\ &\quad\times E(s_0, s'_h)\exp(-i\eta' s'_h\sin\theta_2)\,{\rm d}s'_h.\end{aligned} \qquad (30)$$

This result in a Cartesian system of coordinates is

$$\begin{aligned}E^c_h(x, z) &= \exp[-(i\pi/\lambda)(\chi_0 - \alpha_h)(z/\sin\theta_2)]\\ &\quad\times (i\pi\chi_h C/\lambda\sin\theta_2)\int_z^l E[x-(z'-z)\cot\theta_2, z']\\ &\quad\times \exp\{-i\mathbf{h}\langle\mathbf{u}[x-(z'-z)\cot\theta_2, z']\rangle\}\\ &\quad\times \exp(+i\eta' z')\,{\rm d}z'.\end{aligned} \qquad (31)$$

Expression (31) agrees with the result obtained in another way by Holý *et al.* (1992).

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