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Application of the 'lamellar crystal' approach to study X-ray interbranch scattering by a bent crystal

M. B. Shevchenko

Institute for Metal Physics, National Academy of Sciences of the Ukraine, 36 Vernadsky Street, 03680 Kiev-142, Ukraine. Correspondence e-mail: mish@imp.kiev.ua

The amplitudes of new and normal wavefields are obtained in the case of a slightly bent crystal using the 'lamellar crystal' approach. The physical mechanism of interbranch interaction, which proceeds from this approach, is interpreted in a simple physical manner. The fundamental set of the differential equations is derived to study interbranch scattering within the new representation called the 'eikonal representation'. It is supposed that, in the case of strong bending, an interbranch multiple process may be considered as a resonance one.

1. Introduction

As is well known, the process of interbranch scattering is activated considerably in the case of X-ray dynamical diffraction by a strongly deformed crystal. Such an idea was first given by Penning (1966) and was used by Authier (1967) to explain empirically some features of dislocation images on X-ray section topographs. This phenomenon contradicts the ray theory and occurs when the eikonal approximation (Kato, 1964) becomes invalid. In this connection, the rigorous solution of Takagi's equations was obtained by Katagawa & Kato (1974) and Chukhovskii & Petrashen' (1977) in the case of a uniform strain gradient. With the help of this solution, interbranch scattering was presented in terms of the Green functions which describe the influence of a single point P_0 (usually on the entrance surface) at another point P (usually on the exit surface) (Balibar *et al.*, 1983). However, further study of interbranch scattering is of actual interest; this is due mainly to the extensive use of strongly deformed crystals in advanced X-ray applications. Moreover, these investigations would be of interest to improve the diagnosis of a real crystal, which is a serious problem in the case of combined defects in particular (Kato, 1996). In the present paper, the 'lamellar crystal' approach is applied to examine the phenomenon of interbranch scattering. Such an approach developed by Darwin (1914*a*,*b*) and Zachariasen (1967) was also used by Authier (1961) and Kato (1963) to investigate the propagation of X-rays in deformed crystals. This model was applied to X-ray and neutron diffraction to calculate the rocking curves (Albertini *et al.*, 1976; Erola *et al.*, 1990; Zhong *et al.*, 2003) and to the study of bent monochromators (Egert & Dachs, 1970) as well. At the same time, based on this approach, we can describe the physical mechanism of appearance of the intensive new wavefields predicted by Authier & Balibar (1970) and simulated by Balibar *et al.* (1975), by means of simple physical considerations. The fundamental set of differential equations is derived to examine interbranch scattering by a bent crystal with a uniform strain gradient within this new representation. In addition, new considerations concerning this phenomenon are proposed in the case of a strong bending, which might be helpful for the further development of the dynamical theory of X-ray diffraction by a deformed crystal.

2. General concepts

Using a lamellar crystal as a model for an actual bent crystal is commonly based on the division of the crystal into lamellae parallel to the surface, which have a gradually increasing tilt angle corresponding to the bend of the crystal. In the case of strong deformations, the thickness of the lamella is often taken such that the misorientation angle between two successive lamellae is equal to the Darwin width of the reflection. However, to develop our approach, which would be valid for any strength of deformation, we give up the latter assumption. Instead, we assume that the thickness of the lamellae is so small that the wavefields excited within them can be approximated by plane waves. In doing so, we consider a homogeneously bent crystal where the displacement vector $\mathbf{u}$ is parallel to the entrance surface and depends only on the depth in the crystal z. Consequently, the amplitudes of the transmitted and the diffracted waves $D_{0,g}$ excited in any non-absorbing lamella have the following form in a transmission symmetric case

$$D_0(z) = A^+(l)\exp\left[\frac{i\pi}{\xi_g}(\eta_l + q_l)z\right] + A^-(l)\exp\left[\frac{i\pi}{\xi_g}(\eta_l - q_l)z\right] \quad (1)$$

$$D_g(z) = B^+(l)\exp\left[\frac{i\pi}{\xi_g}(-\eta_l + q_l)z\right] + B^-(l)\exp\left[-\frac{i\pi}{\xi_g}(\eta_l + q_l)z\right]. \quad (2)$$

Here, $z_l \leq z \leq z_{l+1}$, where $l = 0, 1, 2, \ldots$, and the coordinates z_l, z_{l+1} correspond to the front and rear surfaces of the $(l+1)$th lamella, respectively; η_l is the normalized deviation parameter; $q_l = (1 + \eta_l^2)^{1/2}$ and ξ_g is the X-ray extinction length. To avoid intermediate phase contributions during the further calculations that do not influence the final results, amplitudes $A^{\pm}(l)$ are numbered so as to specify the amplitudes before the crystal by $A^{\pm}(0)$. In addition, we suggest that wavefields with amplitudes $A^{\pm}(l)$ are related to the lth lamella, in order that the numbering of lamellae runs from 1.

In fact, expressions (1) and (2) can be considered as the appropriate solutions of Takagi's equations, expressed as combinations of the two wavefields of amplitudes $A^{\pm}$ and $B^{\pm}$, where the + and the − signs correspond to the upper and lower branches of the local dispersion surface, respectively. Since the new wavefields formed due to interbranch scattering increase with increasing deformation, the contribution of the interbranch scattering of the wavefields can be accumulated rapidly with growing crystal thickness. Therefore, to take into account this process correctly, we consider the X-ray dynamical diffraction within 'lamellae', in spite of the fact that their thickness may be significantly less than the X-ray extinction length. Thus, X-ray scattering by the lamellar bent crystal takes place in the manner shown in Fig. 1. In this figure, $\mathbf{k}_0^{\pm}$ and $\mathbf{k}_g^{\pm}$ are the wavevectors of the transmitted and diffracted waves; $\mathbf{n}$ is the normal to the entrance surface and $l+1$, $l+2$, ... denote the lamellar slices. It should be noted that each of the four waves $\mathbf{k}_{0,g}^{\pm}$ formed in the $(l+2)$th lamella can be divided into two terms shown in Fig. 1 separately and marked in different ways. The terms marked by one dash constitute the contributions to the wavefields excited in the $(l+1)$th lamella, which are due to dynamical diffraction of the waves $\mathbf{k}_0^{+}(l)$ or $\mathbf{k}_g^{+}(l)$. At the same time, we mark the contributions associated with dynamical diffraction of the waves $\mathbf{k}_0^{-}(l)$ or $\mathbf{k}_g^{-}(l)$ by two dashes. We will assume also that the wavefields and their first derivatives are continuous on crossing boundaries between lamellae. Then, the basis sets of recurrent equations for amplitudes of the transmitted wave $A^{\pm}$ follow from (1) in accordance with the sketch drawn in Fig. 1.

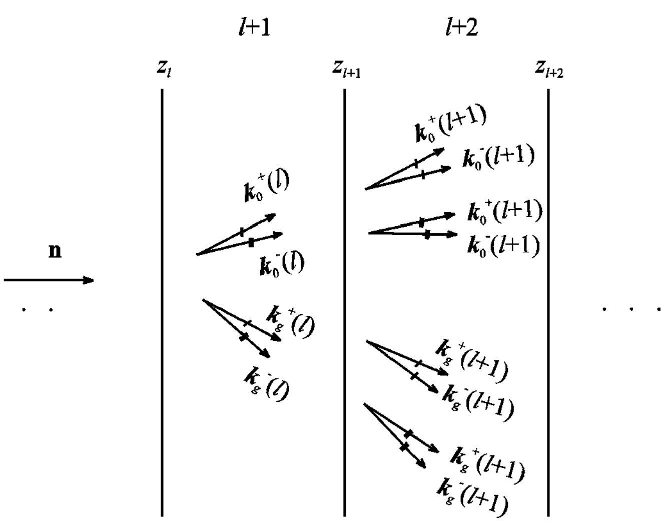

Figure 1
X-ray dynamical diffraction in a lamellar bent crystal.

$$
\begin{aligned}
A^{+}(l+1) = {} & \frac{A^{+}(l)}{2q_{l+1}}[(\eta_l + q_l) - (\eta_{l+1} - q_{l+1})] \\
& \times \exp\left[\frac{i\pi}{\xi_g}(\eta_l - \eta_{l+1} + q_l - q_{l+1})z_{l+1}\right] \\
& + \frac{A^{-}(l)}{2q_{l+1}}[(\eta_l - q_l) - (\eta_{l+1} - q_{l+1})] \\
& \times \exp\left[\frac{i\pi}{\xi_g}(\eta_l - \eta_{l+1} - q_l - q_{l+1})z_{l+1}\right]
\end{aligned} \quad (3)
$$

$$
\begin{aligned}
A^{-}(l+1) = {} & \frac{A^{-}(l)}{2q_{l+1}}[(\eta_{l+1} + q_{l+1}) - (\eta_l - q_l)] \\
& \times \exp\left[\frac{i\pi}{\xi_g}(\eta_l - \eta_{l+1} - q_l + q_{l+1})z_{l+1}\right] \\
& + \frac{A^{+}(l)}{2q_{l+1}}[(\eta_{l+1} + q_{l+1}) - (\eta_l + q_l)] \\
& \times \exp\left[\frac{i\pi}{\xi_g}(\eta_l - \eta_{l+1} + q_l + q_{l+1})z_{l+1}\right].
\end{aligned} \quad (4)
$$

As appears also from (1) and (2), analogous equations for the amplitudes of the diffracted waves $B^{\pm}$ may be obtained from (3) and (4) by replacing $\eta_l \rightarrow -\eta_l$. Such a form of recurrent equations is advantageous to study interbranch scattering because the contributions of the interbranch and into-a-branch processes are separated and expressed in the different terms here. Obviously, the first terms on the right-hand sides of (3) and (4) describe into-a-branch scattering and the second terms interbranch scattering.

In the lamellar crystal approach, analytical description of interbranch scattering effects may be simplified by introducing a new representation of the dynamical diffraction by a bent crystal. Within this representation, hereafter called the 'eikonal representation', we will consider the amplitudes $D_{0,g}$ as superpositions of the modulated normal (*i.e.* predicted by the eikonal theory) wavefields. Then, we should extract into-a-branch contributions from amplitudes $A^{\pm}(l)$ to determine the modulation amplitudes. It is worth observing that concepts presented by Shevchenko & Pobydaylo (2003) may be used as physical motivation to devise such a representation. Indeed, based on the quantum-mechanical analogy of X-ray dynamical diffraction by a deformed crystal, in this work it was suggested that interbranch scattering may be similar to a beating transition between close quantum levels in the case of the violation of adiabatic invariance. This implies amplitude and phase modulation of the normal wavefields due to interbranch transitions, which is taken into account within the eikonal representation. In subsequent sections, we will exploit this representation extensively and obtain new fundamental equations that correspond to the eikonal representation and are suitable for the study of interbranch scattering.

3. The slightly bent crystal case

Examination of X-ray dynamical diffraction by a slightly deformed crystal is of great interest to test any theoretical approach. From this viewpoint, we will apply a lamellar crystal approach to study interbranch scattering by a weakly bent crystal. In this case, the terms on the right-hand sides of (3) and (4), which describe this process, must be so small that they may be neglected in the eikonal approximation of the X-ray dynamical theory. Then, assuming that the thickness of a lamella is sufficiently small, we found the analytical solutions of the recurrent equations with the help of the procedure developed in Appendix *A*. The expression for amplitude D_0 that proceeds from this solution is identical with the one corresponding to the eikonal approach.

To specify interbranch scattering, we introduce the amplitudes of new wavefields $A^{\pm}_{\rm New}$. It is natural to define them in the following manner:

$$A^{\pm}(l) = A^{\pm}_N(l) + A^{\pm}_{\rm New}(l), \qquad (5)$$

where $A^{\pm}_N(l)$ are eikonal approximations of the wave amplitudes. Clearly, $|A^{\pm}_N| \gg |A^{\pm}_{\rm New}|$ in the case of the slightly bent crystal. Bearing this in mind, we insert (5) into (3) and (4), after that we can get the following equations for amplitudes $A^{\pm}_{\rm New}$:

$$A^{\pm}_{\rm New}(l+1) = A^{\pm}_{\rm New}(l) f(\pm q_l, \pm q_{l+1}) + A^{\mp}_N(l) f(\mp q_l, \pm q_{l+1}). \qquad (6)$$

Here functions

$$f(q_l, q_{l+1}) = \frac{1}{2q_{l+1}}[(\eta_l + q_l) - (\eta_{l+1} - q_{l+1})] \times \exp\left[\frac{i\pi}{\xi_g}(\eta_l - \eta_{l+1} + q_l - q_{l+1}) z_{l+1}\right].$$

To consider interbranch processes within the eikonal representation, we extract the fraction equal to an into-a-branch contribution out of the amplitudes $A^{\pm}_{\rm New}(l)$. Such a contribution is described by expression (23) given in Appendix *A*. Consequently, we should take amplitudes $A^{\pm}_{\rm New}(l)$ in the form

$$A^{\pm}_{\rm New}(l) = \tilde{A}^{\pm}_{\rm New}(l) \prod_{n=0}^{l-1} f(\pm q_n, \pm q_{n+1}), \qquad (7)$$

where $\tilde{A}^{\pm}_{\rm New}(l)$ are interbranch components of the modulation amplitudes $\tilde{A}^{\pm}(l)$, by means of which the amplitudes $A^{\pm}(l)$ are expressed in terms of eikonal representation. Taking into account expressions (7) and (23), we rewrite (6) as follows:

$$\Delta\tilde{A}^{\pm}_{\rm New}(l) = A^{\mp}_N(0) \frac{f(\mp q_l, \pm q_{l+1})}{f(\pm q_l, \pm q_{l+1})} \prod_{n=0}^{l-1} \frac{f(\mp q_n, \mp q_{n+1})}{f(\pm q_n, \pm q_{n+1})}. \qquad (8)$$

Here $\Delta\tilde{A}^{\pm}_{\rm New}(l) = \tilde{A}^{\pm}_{\rm New}(l+1) - \tilde{A}^{\pm}_{\rm New}(l)$. To reduce (8), we substitute the approximate expressions (24) for functions $f(\pm q_n, \pm q_{n+1})$ under the product symbol and take into consideration the following equality:

$$\begin{aligned}(q_0 - q_1)z_1 + (q_1 - q_2)z_2 + \ldots + (q_{l-2} - q_{l-1})z_{l-1} + (q_{l-1} - q_l)z_l \\ = q_0(z_1 - z_0) + q_1(z_2 - z_1) + \ldots + q_{l-1}(z_l - z_{l-1}) - q_l z_l, \quad (9)\end{aligned}$$

where the point $z_0 = 0$ corresponds to the entrance surface. Grouping the phase terms in (8) according to (9), we have

$$\Delta\tilde{A}^{\pm}_{\rm New}(l) = A^{\mp}_N(0) \frac{(\eta_l \mp q_l) - (\eta_{l+1} \mp q_{l+1})}{(\eta_l \pm q_l) - (\eta_{l+1} \mp q_{l+1})} \exp\left[\pm \sum_{n=0}^{l-1} \frac{\Delta\eta_n}{q_n}\right] \times \exp\left[\mp \frac{2i\pi}{\xi_g}\left(\sum_{n=0}^{l-1} q_n \Delta z_n + q_l \Delta z_l\right)\right]. \qquad (10)$$

Here, $\Delta z_n = z_{n+1} - z_n$ and $\Delta\eta_n = \eta_{n+1} - \eta_n$. If we let $\Delta z_n \to 0$, it is possible to replace the summation over n by integration over z and modify the multiplier preceding the exponential factors to the form $\eta'(z)(-q \pm \eta)\,{\rm d}z/(2q^2)$. We will suppose that the displacement field $u(z) = \alpha z^2/(2R)$, where R and α are the radius of curvature (defined positive) and the constant describing the deformation, respectively. It is easy to find the derivative $\eta'(z) = \alpha g \xi_g/(2\pi R)$ in this case. Thus, one can obtain from (10) after some straightforward manipulation

$${\rm d}\tilde{A}^{\pm}_{\rm New}(z) = -\frac{\varepsilon\pi}{\xi_g} A^{\mp}_N(0) \frac{\exp\left[\mp(2i\pi/\xi_g)\int_0^z q(z)\,{\rm d}z\right]}{2q^2(z)[\omega \pm (1+\omega^2)^{1/2}]}{\rm d}z. \qquad (11)$$

Here $\varepsilon = \alpha g \xi_g^2/(2\pi^2 R)$ and $\omega = g\xi_g \Delta\theta_{\rm in}/(2\pi)$, where the departure of the incident plane wave from Bragg's law is $\Delta\theta_{\rm in} < 0$. By means of integration, we can derive from (11) the following expressions for $\tilde{A}^{\pm}_{\rm New}$:

$$\tilde{A}^{\pm}_{\rm New}(z) = -\frac{\varepsilon\pi}{\xi_g} \frac{A^{\mp}_N(0)}{\omega \pm (1+\omega^2)^{1/2}} \int_0^z \frac{{\rm d}\zeta}{2q^2(\zeta)} \exp\left[\mp \frac{2i\pi}{\xi_g} \int_0^\zeta q(t)\,{\rm d}t\right]. \qquad (12)$$

Supposing weak bending such that $\varepsilon \ll 1$, integration in (12) may be carried out in an asymptotic way (see Appendix *B*). Then, the amplitudes $\tilde{A}^{\pm}_{\rm New}$ have the form

$$\tilde{A}^{\pm}_{\rm New} \approx \frac{\exp(-2/\varepsilon)}{\omega \pm (1+\omega^2)^{1/2}} \exp\left(\mp\frac{i}{\varepsilon}\{-\omega(1+\omega^2)^{1/2} + \ln[-\omega + (1+\omega^2)^{1/2}]\}\right). \qquad (13)$$

It is necessary to remark that the same results were obtained by Chukhovskii (1980*b*) with the help of the asymptotes of the rigorous solution. One can also obtain it by considering a bent crystal as a crystal sliced in many lamellae. Obviously, this fact verifies the correctness of the general concepts developed above within the lamellar crystal approach.

4. The fundamental equations of dynamical theory in eikonal representation

To study interbranch scattering in the case of a crystal with an arbitrarily strong bending, the new fundamental equations corresponding to eikonal representation may be deduced directly from the basic set of recurrent equations. For this purpose, we rewrite equations (3) and (4) in the form

$$A^{\pm}(l+1) = f(\pm q_l, \pm q_{l+1}) A^{\pm}(l) + f(\mp q_l, \pm q_{l+1}) A^{\mp}(l). \qquad (14)$$

It is clear that, similarly to amplitudes of new wavefields $A^{\pm}_{\rm New}$, amplitudes $A^{\pm}(l)$ can be expressed in terms of the eikonal representation with the help of relations

$$A^{\pm}(l) = \tilde{A}^{\pm}(l) \prod_{n=0}^{l-1} f(\pm q_n, \pm q_{n+1}). \quad (15)$$

Inserting (15) into (14) and introducing $\Delta\tilde{A}^{\pm}(l) = \tilde{A}^{\pm}(l+1) - \tilde{A}^{\pm}(l)$, we can rearrange equations (14) as follows:

$$\Delta\tilde{A}^{\pm}(l) = \frac{f(\mp q_l, \pm q_{l+1})}{f(\pm q_l, \pm q_{l+1})} \tilde{A}^{\mp}(l) \prod_{n=0}^{l-1} \frac{f(\mp q_n, \mp q_{n+1})}{f(\pm q_n, \pm q_{n+1})}. \quad (16)$$

Using the same considerations that were applied to expressions (10) in the previous section, we can derive from (16) the following differential equations for $\tilde{A}^{\pm}(z)$:

$$\frac{\mathrm{d}\tilde{A}^{\pm}(z)}{\mathrm{d}z} = -\frac{\tilde{A}^{\mp}(z) \exp[\mp(2i\pi/\xi_g) \int_0^z q(z)\,\mathrm{d}z]}{2q^2(z)[\omega \pm (1+\omega^2)^{1/2}]} \frac{\varepsilon\pi}{\xi_g}. \quad (17)$$

These equations are valid for any strength of deformation and describe the transfer of energy between the wavefields associated with the different branches of the dispersion surface and forming the transmitted beam. As was noticed above, the value η_l for the transmitted wave is opposite in sign to the appropriate local deviation parameter for the diffracted wave. Hence, the differential equations for the amplitudes $\tilde{B}^{\pm}(z)$ relating to the eikonal representation can be obtained by replacing R by $-R$ and ω by $-\omega$ in equations (17). It should also be observed that equations (17) can be transformed into inhomogeneous differential equations for $\tilde{A}^{\pm}_{\mathrm{New}}(z)$. It is necessary to make the substitution $\tilde{A}^{\pm}(z) = \tilde{A}^{\pm}_{\mathrm{New}}(z) + A^{\pm}(0)$ in (17), which follows from definition (5) in the limit $\Delta z_l \to 0$.

It is worth remarking that, contrary to Takagi's equations, describing both into-a-branch and interbranch scattering, only the latter process is considered by equations (17). For this reason, comparing the eikonal representation and the modulated waves corresponding to Takagi's equations, one can point out an analogy with the quantum-physics representations. Indeed, if the characters of into-a-branch and interbranch scattering are taken into account, it is relevant to associate these processes with nonperturbation and perturbation parts of an effective Hamiltonian, respectively. Then, the Schrödinger and interaction representations will correspond to the modulated waves and the eikonal ones, respectively. This analogy might be of interest to study X-ray dynamical diffraction by a deformed crystal with the aid of the methods developed within the quantum representations.

5. Interbranch multiple scattering of X-rays by strongly bent crystal

In the previous calculations of the amplitudes of new wavefields propagating in a slightly bent crystal, we did not take into account dynamical interchange between the waves $\tilde{A}^{\pm}$. At the same time, considering interbranch scattering as a multiple process, it is natural to suggest that multiple interbranch scattering is intensified significantly with increasing deformations. Obviously, in this case, we must employ equations (17), which have the following form in the vicinity of point z_0:

$$\frac{\mathrm{d}\tilde{A}^{\pm}(z)}{\mathrm{d}z} = -\frac{\varepsilon\pi}{2\xi_g} \varphi^{\pm} \tilde{A}^{\mp} \exp\left(\mp 2i\frac{\pi}{\xi_g} z\right). \quad (18)$$

Here

$$\varphi^{\pm} = \frac{\exp[(\mp 2i\pi/\xi_g) \int_0^{z_0} q(z)\,\mathrm{d}z]}{[\omega \pm (1+\omega^2)^{1/2}]}.$$

It is evident that, by appropriate changes of the amplitudes $A^{\pm}$, equations (18) may be rearranged into the form analogous to Takagi's equations such that their solutions are combinations of the two modes

$$\tilde{A}^{\pm}(z) = c_1^{\pm}(z_0) \exp\left[\frac{i\pi}{\xi_g}(\mp 1 + \mu)z\right] + c_2^{\pm}(z_0) \exp\left[\frac{i\pi}{\xi_g}(\mp 1 - \mu)z\right], \quad (19)$$

where $\mu = [1 + (\varepsilon/2)^2]^{1/2}$ and $c^{\pm}_{1,2}$ are unknown coefficients. Then, comparing expressions (19) and (1), (2), we can treat the distance $\Lambda = \xi_g/(2\varepsilon)$ as the interbranch extinction length. Thus, one can see that interbranch interaction between the waves $\tilde{A}^{\pm}$ results in splitting of the branches of the dispersion surface, which is characterized by the interbranch extinction length. It is reasonable to assert that this dynamical splitting, caused by interbranch interaction, must be taken into account when the following condition is fulfilled:

$$\varepsilon/2 \geq 1. \quad (20)$$

Similarly to the dynamical case of Bragg reflection, one can suppose as well that interbranch scattering may be considered as a resonance dynamical process in the case of strong deformations satisfying (20). Keeping the sketch shown in Fig. 1 in mind, we are able to interpret the physical mechanism of such processes in a simple physical manner. In this connection, we consider the wave $\mathbf{k}_0^+(l)$ excited in the $(l+1)$th lamella. The energy of this wave is partitioned between the waves $\mathbf{k}_0^+(l+1)$ and $\mathbf{k}_0^-(l+1)$ because of the dynamical diffraction of the wave $\mathbf{k}_0^+(l)$ in the $(l+2)$th lamella. However, owing to dynamical diffraction of the wave $\mathbf{k}_0^-(l+1)$ in the $(l+3)$th lamella, some part of the energy of this wave is rescattered back into the wave $\mathbf{k}_0^+$, forming the secondary wave in this direction. As follows from (3) and (4), the amplitude of the primary wave $\mathbf{k}_0^+(l)$ differs from the amplitude of the secondary wave by the following factor near z_0:

$$W = -\left(\frac{\Delta z}{\Lambda}\pi\right)^2 \exp[i\Delta\Phi(z)], \quad (21)$$

where $\Delta\Phi(z) = 2\pi\Delta z/\xi_g$ is the phase shift between these waves. As appears from (21), the secondary beam may modify the amplitude of the primary one considerably when condition (20) is valid. This means that constructive interference of the secondary waves forming the new wavefield takes place, owing to which its amplitude increases significantly. On the other hand, the resulting amplitude of the secondary waves accumulates in the lamellae in a significantly slow way in relation to the destructive phase shift between them, for weak bending with $\varepsilon/2 \ll 1$. For this reason, these waves interfere destructively and the intensity of the new wavefield is small in comparison with that of the normal one. In this case, the amplitudes of the new wavefields identical with (13) may be obtained directly from the set of differential equations (17) by passing to the limit $\varepsilon \to 0$.

It is easy to see that the mechanism of interbranch interaction is similar to that of the dynamical interchange between diffracted and transmitted waves. In both cases, the primary beam should be diffracted a second time, which builds up a twice-diffracted (secondary) beam. However, if we take interbranch scattering into account, it is necessary to consider both diffraction processes as dynamical ones. It follows from this that interbranch interaction will be maximal at the tops of the dispersion hyperbolas, where the most suitable conditions for diffraction are realized. Clearly, owing to an increase of deviation parameter, interbranch interchange will decrease far from z_0. Moreover, the diffracting mechanism of interbranch scattering implies that the interbranch process should be effective inside the range Δz, within which dynamical diffraction of X-rays by a bent crystal takes place. Considering homogeneous bending, it is easy to estimate that $\Delta z \approx R\Psi_D$, where Ψ_D is the angular half-width of the dynamical rocking curve. It is important to note that the value Δz turns out to satisfy the relation $\Delta z \approx \Lambda$ and decreases with decreasing radius R, such that $\Delta z \ll \xi_g$ for a deformation exceeding the limits of the eikonal approximation considerably. Therefore, in the case of strong deformation, interbranch transitions occur in the neighborhood of z_0, which will be contracted with increasing deformation. These facts agree with data from computer experiments, which may be found in a review (Gronkowski, 1991).

Thus, taking into account the multiple character of interbranch scattering, we can introduce the interbranch extinction length Λ and consider such a phenomenon as a resonance one in the case of strong bending. It is worth paying attention to the fact that the value Λ can be controlled by the variation of deformation. When the condition $\Lambda \approx \xi_g$, equivalent to $\varepsilon/2 \approx 1$, is attained in such a way, the eikonal approximation becomes invalid and the generation of the intensive new wavefields takes place (see Authier, 2001). In this case, based on the considerations given above, it is possible to suppose that the resonance increase of interbranch processes should begin as well. In this connection, one may suggest that additional study of this point would be of interest to obtain a deep insight into X-ray dynamical diffraction phenomena in deformed crystals.

6. Conclusions

1. With the application of the lamellar crystal approach to a slightly bent crystal, the amplitudes of the new wavefields and the normal ones corresponding to the eikonal approximation were calculated.

2. The fundamental set of the differential equations was derived from the basic sets of recurrence equations by going to the limit of infinitesimal thickness of a lamella. These equations describe interbranch scattering as dynamical interchange of the modulated normal wavefields, corresponding to different branches of the dispersion surface and given in terms of the new representation called the eikonal representation.

3. With interbranch scattering considered as a dynamical process, the conjecture about the resonance character of this phenomenon in the case of strong deformation was advanced. The criterion $\Lambda \approx \xi_g$ is the necessary condition to realize it, where Λ is the interbranch extinction length.

4. Based on lamellar crystal considerations, a new treatment for the physical mechanism of interbranch interaction was proposed. In this connection, a 'jump' of the tiepoint from one branch to the other should be associated with the formation of twice dynamically diffracted beams.

APPENDIX *A*

In the case of the eikonal approximation of the X-ray dynamical theory, one can represent sets of recurrent equations for amplitudes $A^{\pm}$ in the form

$$A^{\pm}(l) = A^{\pm}(l-1) f(\pm q_l, \pm q_{l+1}). \tag{22}$$

Equations (22) may be solved by means of successive multiplications of the right-hand sides of these equations. After such a procedure, we have

$$A^{\pm}(l) = A^{\pm}(0) \prod_{n=0}^{l-1} f(\pm q_n, \pm q_{n+1}). \tag{23}$$

Here, we put $\eta_0 = 0$ and $q_0 = 0$. Considering the differences $\Delta\eta_l = \eta_{l+1} - \eta_l$ and $\Delta q_l = q_{l+1} - q_l$ to be sufficiently small, we approximate the functions $f(\pm q_l, \pm q_{l+1})$ by the following exponents:

$$f(\pm q_l, \pm q_{l+1}) = \exp\left(\mp \frac{\Delta\eta_l}{2q_{l+1}} - \frac{\Delta q_l}{2q_{l+1}}\right) \times \exp\left[\frac{i\pi}{\xi_g}(\eta_l - \eta_{l+1} \pm q_l \mp q_{l+1}) z_{l+1}\right]. \tag{24}$$

Substituting expressions (24) into (23), we find that the amplitudes $A^{\pm}$ are given by

$$A^{\pm}(l) = A^{\pm}(0) \exp\left[\sum_{n=0}^{l-1} \frac{1}{2q_n}(\mp\Delta\eta_n - \Delta q_n)\right] \times \exp\left[-\frac{i\pi}{\xi_g}(\eta_l \pm q_l) z_l + \frac{i\pi}{\xi_g}\sum_{n=0}^{l-1}(\eta_n \pm q_n)\Delta z_n\right]. \tag{25}$$

Substituting (25) into (1) and considering $z_l \le z \le z_{l+1}$, one can obtain that amplitude $D_0(z_{l+1})$ is the sum of two terms:

$$A^{\pm}(0) \exp\left[\sum_{n=0}^{l-1} \frac{1}{2q_n}\left(\mp \frac{\varepsilon\pi}{\xi_g}\Delta z_n - \Delta q_n\right)\right] \times \exp\left[\frac{i\pi}{\xi_g}(\eta_l \pm q_l)\Delta z_l + \frac{i\pi}{\xi_g}\sum_{n=0}^{l-1}(\eta_n \pm q_n)\Delta z_n\right]. \tag{26}$$

Letting $\Delta z_n \to 0$ and considering the values q and η as functions of the variable z, we replace summation over n in

(26) by integration over z. Then, taking the boundary conditions at $z = 0$ into account, one can obtain the following expression for amplitude $D_0(z)$:

$$D_0(z) = \exp[igu(z)/2] \frac{(1+\omega^2)^{1/2}\cos\Phi(z) - \omega\sin\Phi(z)}{(1+\omega^2)^{1/4}[1+(\omega+\varepsilon\pi z/\xi_g)^2]^{1/4}}, \tag{27}$$

where $\Phi(z)$ is the eikonal function of the following form:

$$\Phi(z) = \frac{1}{2\varepsilon}\Big\{(\omega+\varepsilon\pi z/\xi_g)[1+(\omega+\varepsilon\pi z/\xi_g)^2]^{1/2} - \omega(1+\omega^2)^{1/2} + (1+i\varepsilon)\ln\frac{\omega+\varepsilon\pi z/\xi_g+[1+(\omega+\varepsilon\pi z/\xi_g)^2]^{1/2}}{\omega+(1+\omega^2)^{1/2}}\Big\}. \tag{28}$$

As seen from (27) and (28), these expressions are identical with the appropriate ones corresponding to the eikonal approximation (see Chukhovskii, 1980*a*). It should also be noted that with the help of analogous considerations it is possible to calculate the amplitude of the diffracted wave D_g, which will be identical with the results of the eikonal approach too.

APPENDIX *B*

To determine the amplitudes of new wavefields $\tilde{A}^{\pm}_{\rm New}$ in the case of a slightly bent crystal, we should carry out the following integration:

$$I^{\pm} = -\frac{\varepsilon\pi}{\xi_g}\int\limits_0^z \exp\left[\mp\frac{2i\pi}{\xi_g}\int\limits_0^z q(z)\,{\rm d}z\right]\frac{{\rm d}z}{q^2(z)}. \tag{29}$$

As is easily seen, in the integrand it is convenient to make the substitution $\eta = -\omega(z/z_0 - 1)$, where $z_0 = -\omega\xi_g/(\varepsilon\pi)$, $q(\eta) = (1+\eta^2)^{1/2}$ and, moreover, we take $z \ge z_0$ to account for interbranch scattering near the tops of the dispersion hyperbola. Then, one can get from (29)

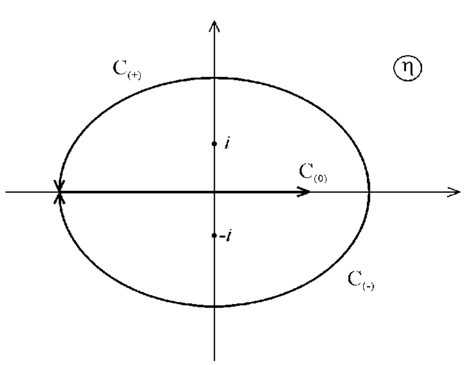

Figure 2
The integration contours for calculation integrals $I^{\pm}$.

$$I^{\pm} = \exp\left[\mp\frac{2i}{\varepsilon}\int\limits_0^{|\omega|} q(t)\,{\rm d}t\right]\int\limits_{\omega}^{\eta}\exp\left[\mp\frac{2i}{\varepsilon}\int\limits_0^{\eta} q(t)\,{\rm d}t\right]\frac{{\rm d}\eta}{q^2(\eta)}. \tag{30}$$

The first multiplier in (30) contains the table integral, which may be taken from Prudnikov *et al.* (1981). At the same time, the second integral in η may be calculated in an asymptotic way under condition $\varepsilon \ll 1$. In this case, the exponential factor in the integrand is an oscillating sharp function and, consequently, integration over the neighborhood is appreciable only at $\eta = 0$. Therefore, one can approximate this factor by $\exp(\mp 2i\eta/\varepsilon)$ and extend the limits of integral to infinities. Then, considering η as a complex variable, we will integrate along the path $C_{(0)} + C_{(-)}$ ($C_{(0)} + C_{(+)}$) enclosing the pole $-i$ ($+i$) for integrals $I^{\pm}$, respectively (see Fig. 2). Placing the contours $C_{(\pm)}$ at infinity, we can neglect integration along them. With this in mind and by calculation of the appropriate residues, it is easy to obtain finally

$$I^{\pm} = \mp\frac{\pi}{2}\exp(-2/\varepsilon)\exp\Big\{\mp\frac{i}{\varepsilon}[-\omega(1+\omega^2)^{1/2} + \ln[-\omega+(1+\omega^2)^{1/2}]\Big\}.$$

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