Diffraction Profiles of Elastically Bent Single Crystals with Constant Strain Gradients, Detailed Theoretical Analysis

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Abstract

We provide detailed derivation of the equations in our paper, "Diffraction Profiles of Elastically Bent Single Crystals with Constant Strain Gradients" in 5 sections. In the 1st section, we derive the classical plane-wave dynamical diffraction theory from first principles. In the 2nd section, we develop the formalism which leads to the recursion equations for dealing with the diffraction problem from strained crystals. In the 3rd section, we show how these recursion equations lead to differential equations that make analytical solutions possible for some cases. In the 4th section, we show the solution of these differential equations for a constant strain gradient, and in the 5th section, we combine this solution with Kato's spherical wave theory and provide the integral equation for the surface intensity distribution in real space which can be evaluated through numerical integration. We also provide analytical equations that approximate this integral for simple calculations.

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1. Plane-wave Dynamical Diffraction Theory for Perfect Crystals

In describing diffraction from perfect crystals using the Ewald-Von Laue formulation, Maxwell's equations can be reduced to the following set of equations (Authier, 2002, Pinsker, 1978)

$$\frac{k_h^2 - K^2}{k_h^2}\vec{D}_h = \sum_l \chi_{h-l}\vec{D}_{l[h]} \tag{1.1}$$

Here $\vec{D}_{l[h]}$ refers to the component of the electric displacement $\vec{D}_l$ parallel to $\vec{D}_h$, $\vec{K}$ is the wave vector in vacuum, $\vec{k}_{0,h}$ are wave vectors in the crystal, χ_h is the h'th Fourier coefficient of the susceptibility and the summations are done over all reciprocal lattice vectors.

Using two-beam approximation (Authier, 2002, Pinsker, 1978), fundamental equations are reduced to two equations:

$$\begin{aligned}\frac{k_0^2 - K^2}{k_0^2}D_0 &= \chi_0 D_0 + C\chi_{\bar{h}} D_h \\ \frac{k_h^2 - K^2}{k_h^2}D_h &= C\chi_h D_0 + \chi_0 D_h\end{aligned}, \tag{1.2}$$

where C, the polarization factor, is equal to $\cos 2\theta$ for π-polarization and 1 for σ-polarization. At the exact Bragg angle calculated from the kinematical theory, the diffracted wavevector $\vec{K}_h$ in vacuum must satisfy:

$$\begin{aligned}\vec{K}_h &= \vec{K}_0 + \vec{h} \\ K_0 &= K_h\end{aligned}. \tag{1.3}$$

From Figure 1, we also have

$$\vec{h} = (h_x, h_z) = h(\sin\varphi, -\cos\varphi)$$
$$\vec{K}_0 = (K_{0x}, K_{0z}) = K(\sin\beta, \cos\beta) \ . \tag{1.4}$$
$$\vec{K}_h = (K_{hx}, K_{hz}) = K(\sin\gamma, -\cos\gamma)$$

There are a number of assumptions that need to be made about the angles in order for the problem to be tractable, first the incidence always occurs from the left side and β and θ are in the range of 0 to $\pi/2$, while φ can vary from $-\pi$ (on the left side of $\vec{n}$) to π (on the right side of $\vec{n}$). The exit angle γ is not independent, but determined by φ and β (or θ). Subscript B is used to refer to parameter values at the exact Bragg condition calculated from the kinematical theory. Combining Equations (1.3) and (1.4), we obtain,

$$K^2 = (h\sin\varphi + K\sin\beta_B)^2 + (-h\cos\varphi + K\cos\beta_B)^2,$$

which yields,

$$h = 2K\cos(\varphi + \beta_B) = 2K\sin\theta_B$$
$$\theta_B = \frac{\pi}{2} - |\varphi + \beta_B| \ . \tag{1.5}$$

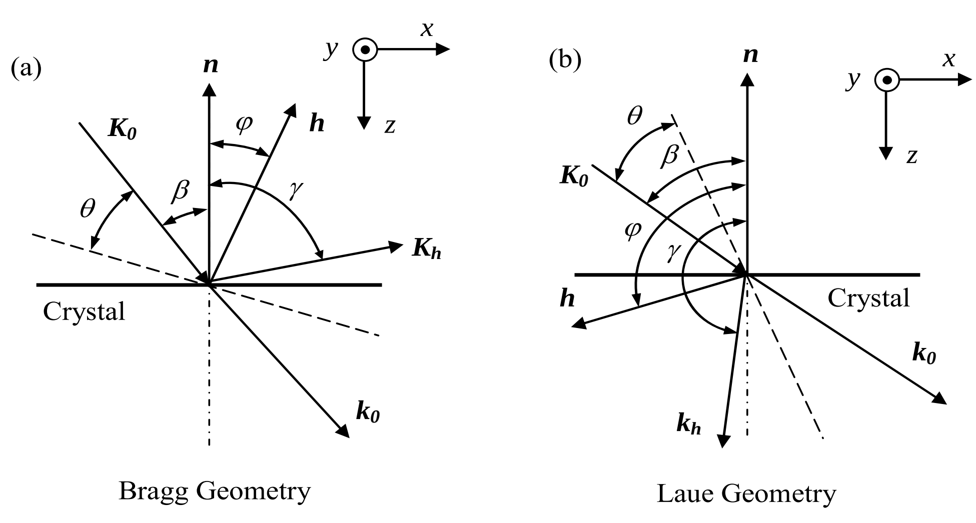

Fig. 1. Diffraction geometries and coordinates system. a) Bragg case, where $|\gamma| < \pi/2$ and $\cos\gamma > 0$; b) Laue case, where $|\gamma| > \pi/2$ and $\cos\gamma < 0$.

The exit angle, γ_B, can be calculated from Equations (1.3) and (1.4), using the equation of the horizontal component of $\vec{K}_h$,

$$\begin{aligned} K\sin\gamma_B &= h\sin\varphi + K\sin\beta_B \\ &= 2K\cos(\varphi+\beta_B)\sin\varphi + K\sin\beta_B \\ &= K\sin(2\varphi+\beta_B) \\ &\Rightarrow \gamma_B = 2\varphi+\beta_B \end{aligned} \quad (1.6).$$

Inside the crystal, the plane wave vectors $\vec{k}_{0,h}$ are not equal to $\vec{K}_{0,h}$. However, the tangential component of the wave vector must be continuous across the interface to satisfy the boundary conditions at the interface,

$$\begin{aligned} \vec{n}\times(\vec{E}_2-\vec{E}_1) &= 0 \\ \vec{n}\times(\vec{H}_2-\vec{H}_1) &= 0 \end{aligned}.$$

Therefore, the *x*-component of the wave vector inside the crystal remains unchanged and we simply need to introduce a small change in vertical component for $\vec{k}_0$,

$$\vec{k}_0 = K(\sin\beta, \cos\beta+\delta). \quad (1.7)$$

The periodicity of χ leads to a Bloch wave solution to the wave equation, which means,

$$\vec{k}_h = \vec{k}_0 + \vec{h} = (K\sin\beta + h\sin\varphi, K\cos\beta - h\cos\varphi + K\delta). \quad (1.8)$$

Now we consider a plane wave incident on the crystal with an incidence angle deviating from the exact Bragg angle θ_B by η. Eq. (1.5) becomes,

$$\theta = \theta_B + \eta = \frac{\pi}{2} - \left|\varphi + \beta_B + \Delta\beta\right|.$$

$$\gamma = \gamma_B + \Delta\gamma.$$

We may write $\Delta\gamma$ in terms of η, by noticing the fact that the diffracted wave outside of the crystal still possesses a wave vector $\vec{K}_h = K(\sin\gamma, -\cos\gamma)$ and its x-component is the same as that of $\vec{k}_h$ in the crystal. Thus, using (1.5) and (1.8), it follows that:

$$K\sin\gamma = h\sin\varphi + K\sin\beta \Rightarrow \sin\gamma \approx 2\sin\theta_B \sin\varphi + \sin\beta_B + \Delta\beta\cos\beta_B .$$

Using Eqs. (1.5) and (1.6), we can prove,

$$2\sin\theta_B \sin\varphi = \cos(\theta_B - \varphi) - \cos(\theta_B + \varphi) = \sin\gamma_B - \sin\beta_B$$

$$\sin(\gamma_B + \Delta\gamma) \approx \sin\gamma_B + \Delta\beta\cos\beta_B \Rightarrow \Delta\gamma = \Delta\beta\cos\beta_B / \cos\gamma_B .$$

Substituting Eqs. (1.7) and (1.8) into Eq. (1.2), and utilizing several trigonometric relations of angles, precise to the first order, one obtains:

$$\frac{k_0^2 - K^2}{k_0^2} \approx 2\delta\cos\beta + \delta^2 \approx 2\delta\cos\beta_B . \quad (1.9)$$

$$\frac{k_h^2 - K^2}{k_h^2} \approx -2\eta\sin 2\theta_B - 2\delta\cos\gamma_B .$$

Here we make several approximations to simplify the expression. First, we assume $|k_{0,h}| \approx K$, so k_0 and k_h in the denominator can be replaced by K. Second, β and γ are large angles so that $\cos\gamma \approx \cos\gamma_B$, $\cos\beta \approx \cos\beta_B$ and the δ^2 term can be ignored. Third, we assume $\sin(\theta_B + \eta) - \sin\theta_B \approx \eta\cos\theta_B$, which is valid when the deviation angle, η, is not very large and θ_B is not close to $\pi/2$. As a result we are not considering the grazing incidence or emergence, nor the case that Bragg angle is close to $\pi/2$. With these approximations the fundamental equation of dynamical diffraction with two-beam condition can be written as:

$$\begin{cases} (\chi_0 - 2\delta\cos\beta_B)D_0 + C\chi_{\bar{h}}D_h = 0 \\ C\chi_h D_0 + (\chi_0 + 2\eta\sin 2\theta_B + 2\delta\cos\gamma_B)D_h = 0 \end{cases} ; C = \begin{cases} 1 & \sigma-\text{polarization} \\ \cos 2\theta & \pi-\text{polarization} \end{cases} . \quad (1.10)$$

For non-trivial solutions the determinant of the coefficient matrix of Eq. (1.10) must be zero, which leads to the dispersion equation,

$$
\begin{aligned}
&-4\delta^2 \cos\beta_B \cos\gamma_B + 2\delta \cos\beta_B [\chi_0(g-1) - 2\eta \sin 2\theta_B] \\
&+ \chi_0^2 + 2\chi_0 \eta \sin 2\theta_B - C^2 \chi_h \chi_{\bar{h}} = 0
\end{aligned}
\tag{1.11}
$$

Eq. (1.11) is a quadric function of δ which has two roots,

$$
\delta^{(j)} = \frac{-v + 2\chi_0 g \mp w}{4\cos\gamma_B}; \qquad j = 1,2, \tag{1.12}
$$

with

$$
\begin{aligned}
&g = \cos\gamma_B / \cos\beta_B \\
&v = (1+g)\chi_0 + 2\eta \sin 2\theta_B \ . \\
&w = \sqrt{v^2 - 4C^2 g \chi_h \chi_{\bar{h}}}
\end{aligned}
$$

g is the geometry factor, which is positive for Bragg geometry and negative for Laue geometry, and v is the deviation parameter. The "$\mp$" sign implies that two wave branches will be excited for both forward-diffracted and diffracted beams. Thus, in general the entire wave field in a perfect crystal is represented by a set of four plane waves. To denote those branches there is one thing needs to be clarified: the complex variable w has two possible values determined by the phase of the complex argument under the square root.

In the Laue case where g is negative, we assume the real component of w is always positive and denote the "-" sign in Eq. (1.12) as branch 1. In the Bragg case where g is positive, to avoid ambiguity, we set a cut line from origin to the positive infinity of the x-axis on the complex plane and restrict the phase of a complex variable to (0, 2π). This means the phase of w will vary within (0, π) and its imaginary part is always positive. By this convention, we denote the "-" sign in Eq. (1.12) as branch 1 and the "+" sign as branch 2. The real part of δ represents refraction and its imaginary part absorption. We shall notice a wave form $\exp(-i2\pi\vec{k} \cdot \vec{r})$ is used in our derivation; as a result a positive $\mathrm{Im}(\delta)$ stands for a wave increasing with depth, while a negative $\mathrm{Im}(\delta)$ stands for a wave decreasing with depth. In the Bragg case ($g > 0$), $\mathrm{Im}[\delta^{(1)}] < 0$ but $\mathrm{Im}[\delta^{(2)}] > 0$, thus, for a semi-infinite crystal branch 2 is physically impossible due to the fact that at infinity the amplitude of branch 2 will be infinit. In the Laue case ($g < 0$), the thickness is finite and $\mathrm{Im}(\delta)$ for both branches have negative values, and both branches will be excited. But when η is very negative only branch 1 is strongly excited, and when η is very positive only branch 2 is strongly excited, according to our definition of branches. Substituting Eq. (1.12) into Eqs. (1.7) and (1.8), we deduce expressions of wave vectors $\vec{k}_0$ and $\vec{k}_h$,

$$\begin{aligned}\vec{k}_0^{(j)} &= K(\sin\beta, \cos\beta + \delta^{(j)}) \approx K(\sin\beta, \cos\beta_B + \frac{\chi_0(g-1) - 2\eta\sin 2\varphi \mp w}{4\cos\gamma_B}) \\ \vec{k}_h^{(j)} &= \vec{k}_0^{(j)} + \vec{h} \approx K(\sin\gamma, -\cos\gamma_B + \frac{\chi_0(g-1) - 2\eta\sin 2\varphi \mp w}{4\cos\gamma_B})\end{aligned} \quad , \quad j = 1,2$$

with $\gamma = \gamma_B + \Delta\beta / g$. (1.13)

Substituting the expressions of δ given in Eq. (1.12) into Eq. (1.10), one obtains the diffraction coefficient in terms of deviation angle η,

$$c^{(j)} = \frac{D_h^{(j)}}{D_0^{(j)}} = \frac{-v \mp w}{2gC\chi_{\bar{h}}}, \qquad j = 1,2 . \tag{1.14}$$

Combining Eq. (1.14) with Eq. (1.12) is still insufficient to describe the whole wave field because we don't know the fraction of energy taken by each branch. By applying proper boundary conditions, for example, $D_0^{(1)} + D_0^{(2)} = 1$ and $D_h^{(1)} + D_h^{(2)} = 0$ for Laue geometry, we can solve the amplitudes of all these four plane waves. Consequently, the entire wave field inside a perfect crystal corresponding to an incident plane wave is expressed as the superposition of all excited waves,

$$\vec{D}(\vec{r}) = \sum_{j=1,2} \{\vec{D}_0^{(j)} \exp[-i2\pi\vec{k}_0^{(j)} \cdot \vec{r}] + \vec{D}_h^{(j)} \exp[-i2\pi\vec{k}_h^{(j)} \cdot \vec{r}]\} \tag{1.15}$$

2. Recursion Relations for Strained Crystals

Using some simple considerations, we can extend the classical theory to a strained case. The basic idea is to consider the dynamical diffraction of a very thin layer in a distorted crystal (Fig. 2), and treat the strain within this layer as constant and the layer as still perfect. The four plane waves in Fig. 2 (two for reflection and two for transmission) with constant amplitudes on the top boundary of the thin layer propagate through the thickness and then reach the bottom boundary. If the wave amplitudes of these four plane waves at one boundary are known, taking into account the phase change and absorption which can be obtained from the classical theory, one can obtain the total diffracted and forward-diffracted wave amplitudes at the other boundary, leading to the recurrence relations for reflection and transmission. All results obtained in classical dynamical diffraction theory are applicable to this thin layer except *local* values must be used for all parameters to reflect the change of material properties. The concept of a local dispersion equation is introduced as in the optical theory of dynamical diffraction (Authier, 2002), which describes the ray trajectory inside a strained crystal. In our model because the entire wave field, not the individual branch is considered, the “interbranch scattering” problem (Balibar *et al.*, 1983) for large strain gradients, which refers to the energy interchange between two branches, is solved automatically, and the limitation of very small deformation field in optical theory is eliminated.

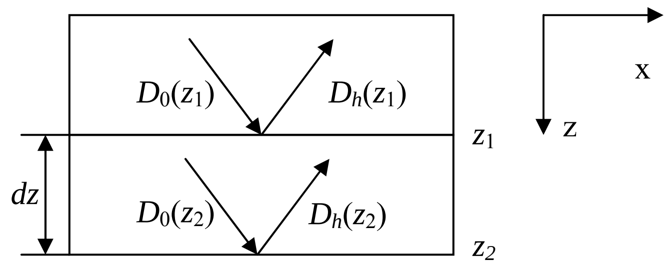

Fig. 2. Dynamical diffraction on a thin layer with thickness *dz*. Inside the layer the strain is treated as constant.

Usually, a deformation field consists of rotations and changes of the spacing of the lattice planes, and their effects are reflected by the local deviation angle, η, which is the difference in the incidence angle from the local exact Bragg angle. A strain will cause a shift of the local Bragg angle that can be calculated from Bragg's law, and a rotation angle $\delta\theta$ will cause a change in the local incidence angle. Thus, the deviation angle can be written as:

$$\eta = \eta_0 + \delta\theta + \varepsilon \tan\theta_B\,, \qquad (2.1)$$

where η_0 is the value of η for the unstrained crystal. Inside a very thin layer, dynamical diffraction theory of perfect crystals still holds and the forward-diffracted and diffracted waves are still written in the form of Bloch waves:

$$\begin{aligned} D_h(\vec{r}) &= D_h^{(1)} \exp[-i2\pi\vec{k}_h^{(1)} \cdot \vec{r}] + D_h^{(2)} \exp[-i2\pi\vec{k}_h^{(2)} \cdot \vec{r}] \\ D_0(\vec{r}) &= D_0^{(1)} \exp[-i2\pi\vec{k}_0^{(1)} \cdot \vec{r}] + D_0^{(2)} \exp[-i2\pi\vec{k}_0^{(2)} \cdot \vec{r}]\,. \\ \vec{k}_h^{(j)} &= \vec{k}_0^{(j)} + \vec{h}'; \qquad j = 1,2 \end{aligned} \qquad (2.2)$$

Here we use $\vec{h}'$ to represent the *local* reciprocal lattice vector, which is a function of depth, *z*. By using the local values, we can find the diffraction coefficient $c^{(j)}$ and wave vectors $\vec{k}_0^{(j)}$ and $\vec{k}_h^{(j)}$ of each branch from Eq. (1.13) and (1.14). Usually, the diffraction ratio D_h/D_0 is what we want to know, where both D_h and D_0 are the sum of two wave branches. By substituting Eq. (1.13) into Eq. (2.2), we can obtain the expression of the overall diffraction coefficient,

$$\frac{D_h}{D_0} = \frac{\exp[-i2\pi(\vec{K}_0+\vec{h}')\cdot\vec{r}]\{D_h^{(1)}\exp[-i2\pi K\delta^{(1)}z]+D_h^{(2)}\exp[-i2\pi K\delta^{(2)}z]\}}{\exp(-i2\pi\vec{K}_0\cdot\vec{r})\{D_0^{(1)}[-i2\pi K\delta^{(1)}z]+D_0^{(2)}\exp[-i2\pi K\delta^{(2)}z]\}}$$
$$= \exp(-i2\pi\vec{h}'\cdot\vec{r})\frac{D_h^{(1)}\exp(i\Phi z/2)+D_h^{(2)}\exp(-i\Phi z/2)}{D_0^{(1)}\exp(i\Phi z/2)+D_0^{(2)}\exp(-i\Phi z/2)}$$

with $\Phi = K\pi\, w/\cos\gamma_B$.

Because only the vertical components of wave vectors can vary in a deformed crystal, for convenience, we can define a new variable X that solely depends on z,

$$X = \exp(i2\pi\vec{h}'\cdot\vec{r})\frac{D_h}{D_0}. \tag{2.3}$$

X has the same modulus with the true diffraction ratio, but differs it by a phase depending on positions. At boundaries of this layer, we can write:

$$\begin{aligned} X_1 &= \frac{D_h^{(1)}\exp(i\Phi z_1/2)+D_h^{(2)}\exp(-i\Phi z_1/2)}{D_0^{(1)}\exp(i\Phi z_1/2)+D_0^{(2)}\exp(-i\Phi z_1/2)}; \qquad z = z_1 \\ X_2 &= \frac{D_h^{(1)}\exp(i\Phi z_2/2)+D_h^{(2)}\exp(-i\Phi z_2/2)}{D_0^{(1)}\exp(i\Phi z_2/2)+D_0^{(2)}\exp(-i\Phi z_2/2)}; \qquad z = z_2 \end{aligned}, \tag{2.4}$$

and the subscripts $_1$ and $_2$ of X refer to its value at depth z_1 and z_2. By substituting Eq. (1.14) to Eq. (2.4), we obtain two equations:

$$\begin{aligned} D_0^{(1)} &= \exp(-i\Phi z_1)\frac{X_1-c^{(2)}}{c^{(1)}-X_1}D_0^{(2)}, \\ D_0^{(1)} &= \exp(-i\Phi z_2)\frac{X_2-c^{(2)}}{c^{(1)}-X_2}D_0^{(2)}. \end{aligned} \tag{2.5}$$

After canceling out $D_0^{(1)}$ and $D_0^{(2)}$ on both sides of Eq. (2.5) and plugging in the expressions of the diffraction coefficient, one obtains the recurrence relation for reflection,

$$X_1 = \frac{wX_2 - i(2C\chi_h + vX_2)\tan[\Phi(z_2 - z_1)/2]}{w + i(2gC\chi_{\bar{h}}X_2 + v)\tan[\Phi(z_2 - z_1)/2]}, \tag{2.6a}$$

or

$$X_2 = \frac{wX_1 + i(2C\chi_h + vX_1)\tan[\Phi(z_2 - z_1)/2]}{w - i(2gC\chi_{\bar{h}}X_1 + v)\tan[\Phi(z_2 - z_1)/2]}. \tag{2.6b}$$

This recurrence relation is not a new result. It has been obtained by some authors from integrating the Takagi-Taupin equations for a perfect lamellar of crystal (Halliwell *et al.*, 1984, Bartels *et al.*, 1986), and is implemented in some commercial software, such as RADS[2], which is used for rocking curve simulation of epitaxially grown heterostructures, but our approach gives a very simple and clear derivation of this relation.

The derivation of the recurrence relation for transmission is analogous to that of reflection. The overall forward-diffracted wave is the sum of two excited branches, therefore the ratio of the forward-diffracted wave amplitude at $z = z_2$ to that at $z = z_1$ is written as:

$$\begin{aligned}\frac{D_0(\vec{r}_2)}{D_0(\vec{r}_1)} &= \exp[-i2\pi\vec{K}_0\cdot(\vec{r}_2-\vec{r}_1)]\frac{D_0^{(1)}\exp[-i2\pi\delta^{(1)}z_2] + D_0^{(2)}\exp[-i2\pi\delta^{(2)}z_2]}{D_0^{(1)}\exp[-i2\pi\delta^{(1)}z_1] + D_0^{(2)}\exp[-i2\pi\delta^{(2)}z_1]} \\ &= \exp[-i2\pi\vec{K}'_0\cdot(\vec{r}_2-\vec{r}_1)]\exp[-i\pi K\chi_0(\frac{1}{\cos\beta_B}-\frac{1}{\cos\gamma_B})(z_2-z_1)] \\ &\times\frac{D_0^{(1)}\exp(i\Phi z_2/2) + D_0^{(2)}\exp(-i\Phi z_2/2)}{D_0^{(1)}\exp(i\Phi z_1/2) + D_0^{(2)}\exp(-i\Phi z_1/2)}\end{aligned}, \tag{2.7}$$

with $\vec{K}'_0 = \vec{K}_0 - K\frac{\eta(z)\sin 2\theta_B}{2\cos\gamma_B}\vec{z}$. Using Eqs. (2.5), we obtain the recurrence relation of the transmission at z_1 to its adjacent layer at z_2,

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[2] RADS is a product of Bede Scientific Instruments Ltd.

$$\frac{Y_2}{Y_1} = \frac{w\cos[\Phi(z_2 - z_1)/2] - i(2Cg\chi_{\bar{h}} X_1 + v)\sin[\Phi(z_2 - z_1)/2]}{w} \times \exp[-i\pi K\chi_0(\frac{1}{\cos\beta_B} - \frac{1}{\cos\gamma_B})(z_2 - z_1)], \qquad (2.8a)$$

or

$$\frac{Y_2}{Y_1} = \frac{w}{w\cos[\Phi(z_2 - z_1)/2] + i(2Cg\chi_{\bar{h}} X_2 + v)\sin[\Phi(z_2 - z_1)/2]} \times \exp[-i\pi K\chi_0(\frac{1}{\cos\beta_B} - \frac{1}{\cos\gamma_B})(z_2 - z_1)], \qquad (2.8b)$$

where Y is defined as

$$Y = D_0(\vec{r})\exp(i2\pi\vec{K}'_0 \cdot \vec{r}).$$

The subscripts $_1$ and $_2$ of Y refer to its value at depth z_1 and z_2. We should note that $|X|=|D_h/D_0|$, $|Y|=|D_0|$ and $|XY|=|D_h|$, and the expressions of the true diffracted and forward-diffracted wave with correct phase terms are:

$$\begin{aligned} D_0(\vec{r}) &= Y\exp(-i2\pi\vec{K}'_0 \cdot \vec{r}) \\ D_h(\vec{r}) &= XY\exp[-i2\pi(\vec{K}'_0 + \vec{h}') \cdot \vec{r}] \end{aligned} \qquad (2.9)$$

Combining with Eq. (2.7) and Eq. (2.8), by applying dynamical diffraction theory consecutively on thin slabs with constant strain, we are able to solve the entire x-ray wave field in crystals with heterostructures, misorentation or strain field.

3. Fundamental Differential Equations for Strained Crystals

To find the analytical description of the wave field, generic equations including the misorientation or strain function need to be established. The idea is to reduce the thickness $dz = z_2 - z_1$ of the layer into an infinitesimal thickness and write all functions as Taylor expansions around z. When dz becomes infinitesimal, the approximation up to the first order of dz is always justified, but in practice dz cannot be smaller than the interplanar spacing, d_{hkl}. Thus the approximation up to the first order is equivalent to the statement that the variation of the strain over a range of d_{hkl} is very slow and high order derivatives can be neglected. Consequently, Eq. (2.6a) turns into [if Eq. (2.6b) is used, the result is the same],

$$X(z) \approx \frac{w(X + dzX') - i[2C\chi_h + v(X + dzX')]\Phi dz/2}{w + i[2Cg\chi_{\bar{h}}(X + dzX') + v]\Phi dz/2}.$$

By rearranging terms and neglecting high order terms in *dz*, one obtains the differential equation for diffraction:

$$X' = \frac{iK\pi}{\cos\gamma_B}(Cg\chi_{\bar{h}}X^2 + vX + C\chi_h). \tag{3.1}$$

Very similarly, by expanding Eq. (2.8a) or Eq. (2.8b) as a Taylor series, up to the first order of *dz*, we can deduce,

$$\frac{Y'}{Y} = -i\frac{K\pi}{2\cos\gamma_B}[2Cg\chi_{\bar{h}}X + v + \chi_0(g-1)]. \tag{3.2}$$

By noting $(\ln Y)' = Y'/Y$, we recognize Eq. (3.2) is the equation that relates the local amplitude attenuation of the forward-diffracted wave to the local diffraction ratio *X*. This is the equation of extinction. The weakening effect of transmission due to diffraction is shown clearly by Eq. (3.2). Furthermore, if we differentiate both sides of Eq. (3.2) and substitute into Eq. (3.1), a new equation only involving Y'/Y is derived,

$$(Y'/Y)' + (Y'/Y)^2 = -ia[v' + 2(Y'/Y)\chi_0(g-1)] + a^2[\chi_0^2(g-1)^2 - w^2], \tag{3.3}$$

with $a = K\pi/2\cos\gamma_B$. Since $(Y'/Y)' + (Y'/Y)^2 = Y''/Y$, Eq. (3.3) can also be written as,

$$Y'' + i2a\chi_0(g-1)Y' + \{a^2[w^2 - \chi_0^2(g-1)^2] + iav'\}Y = 0. \tag{3.4}$$

This equation can be further simplified if we set $Y(z) = \exp[-ia\chi_0(g-1)z]U(z)$, which leads to a wave equation in the simple form:

$$U''+(a^2w^2 + iav')U = 0\,, \tag{3.5}$$

and Eq. (3.2) is rewritten as

$$\frac{U'}{U} = -ia(Cg\chi_{\bar{h}}X + v)\,. \tag{3.6}$$

Eqs. (3.1) and (3.5) are the fundamental differential equations of dynamical diffraction on crystals with a one-dimensional strain field, with the incident-plane-wave and two-beam approximations. They are not independent equations, but related by Eq. (3.6), so we only need to solve one equation to obtain the complete set of solutions. We note these differential equations have a similar form to the well-known Howie-Whelan equations in electron diffraction (Diffraction and Imaging Techniques in Material Science, 1978).

4. Analytical Solutions in Symmetric Bragg Case

For simplicity, in the following we only consider symmetric Bragg diffraction and a σ-polarized incident plane wave. Under these conditions the fundamental differential equations we derived in the preceding section are simplified to:

$$X' = i2a(\chi_{\bar{h}}X^2 + vX + \chi_h)\,, \tag{4.1a}$$

$$Y'/Y = -ia(2\chi_{\bar{h}}X + v)\,, \tag{4.1b}$$

$$Y''+(a^2w^2 + iav')Y = 0\,, \tag{4.1c}$$

with

$$a = K\pi / 2\sin\theta_B$$
$$v = 2\chi_0 + 2\eta(z)\sin 2\theta_B \ .$$
$$w = \sqrt{v^2 - 4\chi_h \chi_{\bar{h}}}$$

For a given constant misorientation/strain gradient in the normal direction, we can write the deviation angle as:

$$\eta = \eta_0 + \eta' z \,, \tag{4.2}$$

where η' is a constant. Accordingly, the deviation parameter v will be a linear function of depth *z* too,

$$v(z) = v_0 + v' z \,, \tag{4.3}$$

where v' is a constant and v_0 is the value of v at the entrance surface.

Due to its linearity, Eq. (4.1c) is the one we can find a solution easily. Combined with Eq. (4.1b), the diffraction coefficient *X* can be derived as well. To simplify Eq. (4.1c) we define a new variable *q*,

$$q = \sqrt{\frac{ia}{v'}} v = \begin{cases} \sqrt{\frac{a}{|v'|}} e^{\pi i/4} v & v' > 0 \\ \sqrt{\frac{a}{|v'|}} e^{3\pi i/4} v & v' < 0 \end{cases} . \tag{4.4}$$

Eq. (4.1c) is then transformed to:

$$Y''(q) + (2b + 1 - q^2) Y(q) = 0 \,, \tag{4.5}$$

with $b = \frac{2ia\chi_h \chi_{\bar{h}}}{v'}$. The solution of Eq. (4.5) is a parabolic cylinder function, which is known as a Weber function. To explain the physical meaning of the solution in a better way, we transform Eq. (4.5) to a Hermite equation,

$$\zeta'' - 2q\zeta' + 2b\zeta = 0 \,, \tag{4.6}$$

with $\zeta(q) = \exp(q^2/2)Y(q)$. Eq. (4.6) can be solved using a polynomial series (Arfken & Weber, 1995). Assuming $\zeta(q)$ can be expanded to a series of polynomials,

$$\zeta(q) = \sum_{n=0}^{\infty} C_n q^n \ . \tag{4.7}$$

Substituting the above equation into Eq. (4.6), one obtains a new equation,

$$\sum_{n=0}^{\infty} [C_{n+2}(n+2)(n+1) - C_n(2n-2b)]q^n = 0 \ . \tag{4.8}$$

The sum of the coefficients of terms with same polynomial number *n* must be zero to fulfill Eq. (4.8). This results in the coefficient iteration equation:

$$C_{n+2} = \frac{2n-2b}{(n+2)(n+1)} C_n, \quad n = 0,1,2,3,\dots. \tag{4.9}$$

It is seen that all even coefficients, C_{2n}, can be written in terms of C_0, and all odd coefficients, C_{2n+1}, can be written in terms of C_1. Using C_0 and C_1, we can construct two linearly independent solutions,

$$\begin{aligned}
\zeta_1(q) &= 1 - bq^2 + \frac{b(b-2)}{6}q^4 + \cdots = {}_1F_1(-\frac{b}{2};\frac{1}{2};q^2), \\
\zeta_2(q) &= q(1 + \frac{1-b}{3}q^2 + \frac{(3-b)(1-b)}{30}q^4 + \cdots) = q\,{}_1F_1(\frac{1-b}{2};\frac{3}{2};q^2),
\end{aligned} \tag{4.10}$$

here ${}_1F_1$ is a confluent hypergeometric function.(Andrews, 1985, Magnus *et al.*, 1966, Luke, 1969) The general solution is the linear combination of these two confluent hypergeometric functions,

$$\begin{aligned}
\zeta(q) &= C_0\zeta_1(q) + C_1\zeta_2(q), \\
Y(q) &= e^{-\frac{q^2}{2}}\zeta(q).
\end{aligned} \tag{4.11}$$

In general, the linear combination coefficients are determined by boundary conditions and expressed in complicated forms. Here we consider a special case in which the crystal thickness is infinite. In reality, an infinite thick crystal with a linear strain gradient is physically impossible, but this is a good approximation to the true solution if the crystal thickness is large. Under this assumption the boundary condition for Bragg diffraction can be written as:

$$|Y| \to 0 \text{ if } z \to +\infty . \tag{4.12}$$

According to the definition, q is proportional to z and $|q| \to \infty$ as $z \to \infty$. For an infinitely thick crystal, the boundary condition at infinity requires that the forward-diffracted wave intensity is decreased to zero. When q is very large, in Eq. (4.10) we only need to keep terms with very large n, and approximately, $C_{n+2} / C_n \sim 2/n$, which is equivalent to the expansion coefficients of an exponential function. Thus, if $|q| \to \infty$, the approximate expression of $\zeta(q)$ is:

$$\zeta(q) \sim \exp(q^2),$$

and

$$Y(q) \sim \exp(q^2/2).$$

Because $\mathrm{Re}(q^2) = -2a\chi_{0i}z \to +\infty$ when $z \to +\infty$ (in our derivation, we chose the wave form $\exp(-i2\pi\vec{k}\cdot\vec{r})$, so χ_{0i} is negative), either Y_1 or Y_2 does not converge at infinity and is not the solution. To find the combination coefficients C_0 and C_1 that can construct a function convergent at infinity, we need to study the asymptotic expansions of ζ_1 and ζ_2 around infinity. It is known that for $|x| \to \infty$, the asymptotic expansion of a confluent hypergeometric function is (Slater, 1960):

$$
{}_1F_1(\alpha;\gamma;x) \sim \frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)} e^{\varepsilon\alpha\pi i} x^{-\alpha} \{\sum_{n=0}^{R-1} (-1)^n \frac{(\alpha)_n (1-\gamma+\alpha)_n}{n! x^n} + O(|x|^{-R})\} + \frac{\Gamma(\gamma)}{\Gamma(\alpha)} e^x x^{\alpha-\gamma} \{\sum_{n=0}^{S-1} \frac{(\gamma-\alpha)_n (1-\alpha)_n}{n! x^n} + O(|x|^{-S})\} , \quad (4.13)
$$

for $R,S = 0,1,2,...$, and $\varepsilon = 1$ if $0 < \arg x < \pi$, $\varepsilon = -1$ if $-\pi < \arg x \le 0$. Hence,

$$
\zeta_1(q) \sim \frac{\Gamma(1/2)}{\Gamma(1/2+b/2)} e^{\varepsilon(-b/2)\pi i} q^b \{1 + \sum_{n=1}^{\infty} (-1)^n \frac{(-b/2)_n (1/2-b/2)_n}{n! q^{2n}}\} + \frac{\Gamma(1/2)}{\Gamma(-b/2)} e^{q^2} q^{-b-1} \{1 + \sum_{n=1}^{\infty} \frac{(1/2+b/2)_n (1+b/2)_n}{n! q^{2n}}\} , \quad (4.14a)
$$

$$
\zeta_2(q) \sim \frac{\Gamma(3/2)}{\Gamma(1+b/2)} e^{\varepsilon(1-b)\pi i/2} q^b \{1 + \sum_{n=1}^{\infty} (-1)^n \frac{(1/2-b/2)_n (-b/2)_n}{n! q^{2n}}\} + \frac{\Gamma(3/2)}{\Gamma(1/2-b/2)} e^{q^2} q^{-b-1} \{1 + \sum_{n=1}^{\infty} \frac{(1/2+b/2)_n (1+b/2)_n}{n! q^{2n}}\} . \quad (4.14b)
$$

The second terms on the right side of Eqs. (4.14a) and (4.14b) represents a steeply increasing function as $|q| \to \infty$ and should be canceled to ensure convergence at infinity. This requires a special linear combination of ζ_1 and ζ_2 to construct the solution, which is known as a Hermite function,

$$
\begin{aligned}
Y(q) = e^{-\frac{q^2}{2}} H_b(q) &= e^{-\frac{q^2}{2}} 2^b \sqrt{\pi} [\frac{1}{\Gamma(\frac{1-b}{2})} \zeta_1(q) - \frac{2}{\Gamma(-\frac{b}{2})} \zeta_2(q)] \\
&= e^{-\frac{q^2}{2}} 2^b \sqrt{\pi} [\frac{1}{\Gamma(\frac{1-b}{2})} {}_1F_1(-\frac{b}{2};\frac{1}{2};q^2) - \frac{2q}{\Gamma(-\frac{b}{2})} {}_1F_1(\frac{1-b}{2};\frac{3}{2};q^2)]
\end{aligned} , \quad (4.15)
$$

where Γ represents a gamma function. For a normalized incident beam, a normalization factor is introduced to ensure that $Y(z=0) = 1$,

$$
Y(q) = e^{-\frac{q^2}{2}} H_b(q)/Y_0 \text{ with } Y_0 = e^{-\frac{q_0^2}{2}} H_b(q_0) \text{ and } q_0 = q(0) . \quad (4.16)
$$

If we write q in terms of z and expand q^2, because $\mathrm{Re}(-q^2/2) = (K\pi/\sin\theta_B)\chi_{0i}z$ (χ_{0i} is the imaginary part of χ_0 and is negative in our derivation), the pre-exponential factor actually represents the normal linear photoelectric absorption.

To find the expression of *X*, we utilize the differential formulas of Hermite function (Andrews, 1985),

$$\begin{aligned} \frac{\partial H_b(q)}{\partial q} &= 2bH_{b-1}(q), \\ \frac{\partial H_b(q)}{\partial q} - 2qH_b(q) &= -H_{b+1}(q). \end{aligned} \tag{4.17}$$

By combining with Eq. (4.1b), the expressions of X is derived,

$$\frac{Y'}{Y} = -iav + 2b\sqrt{iav'}\frac{H_{b-1}(q)}{H_b(q)}, \tag{4.18}$$

$$X = -2\chi_h\sqrt{ia/v'}\frac{H_{b-1}(q)}{H_b(q)}. \tag{4.19}$$

The right-hand side of Eq. (4.18) consists of two terms; the first one represents the linear photoelectric absorption and the second one represents dynamical attenuation by reflection. Eqs (4.16), (4.18) and (4.19) are the analytical solutions for diffraction on an infinitely thick crystal with a constant strain gradient, and are good approximations for crystals with thickness larger than the penetration depth. We may call this the thick-crystal approximation. The rigorous solutions for a crystal with finite thickness can also be obtained by noting that $H_b(-q)$ is also a solution to Eq. (4.6). For $b \neq 0, \pm1, \pm2, \cdots$, which is the case in dynamical diffraction, $H_b(-q)$ is linearly independent of $H_b(q)$. Thus, the general solution can also be written as:

$$Y(q) = \exp(-q^2/2)[C_1H_b(q) + C_2H_b(-q)]. \tag{4.20}$$

The boundary condition at $z = t$ in the Bragg case requires:

$$X(t) = 0 \Rightarrow C_1 H_{b-1}[q(t)] - C_2 H_{b-1}[-q(t)] = 0\,.$$

So, we deduce:

$$\frac{C_2}{C_1} = \frac{H_{b-1}[q(t)]}{H_{b-1}[-q(t)]} = C_t\,, \tag{4.21}$$

and the exact solution is

$$Y(q) = \exp(-q^2/2)[H_b(q) + C_t H_b(-q)]/Y_0\,, \tag{4.22}$$

with $Y_0 = \exp(-q_0^2/2)[H_b(q_0) + C_t H_b(-q_0)]$ and $q_0 = q(0)$. From Eq. (4.1b), one obtains:

$$X = -2\chi_h \sqrt{ia/v'}\,\frac{H_{b-1}(q) - C_t H_{b-1}(-q)}{H_b(q) + C_t H_b(-q)}\,. \tag{4.23}$$

5. Surface Intensity Distribution for Spherical Incident Wave

a) General Formalism

To obtain the correct expression of the diffracted wave for an incident spherical wave, we follow Kato's spherical-wave theory (Kato, 1960). His method comprises three steps:

i. Expand a spherical wave in terms of a distribution of plane waves with same wave number by means of the Fourier transform.

ii. Apply the plane-wave model for each plane wave component of the spherical wave to obtain the forward-diffracted and diffracted wave amplitude corresponding to this plane wave component.

iii. Obtain the sum of the induced wave amplitudes of all plane-wave components by means of the inverse Fourier transform to obtain the induced wave amplitude caused by the incident spherical wave.

Detailed discussions about Kato's theory can be found in the textbooks by Pinsker (Pinsker, 1978) and Authier (Authier, 2002). Here we give a brief derivation. In real space a scalar wave emitted by a point source can be written as (the time dependent term is dropped)

$$\phi(r) = \frac{\exp(-2i\pi Kr)}{4\pi r}$$

Written as a Fourier transform,

$$\phi(r) = \frac{i}{4\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\exp(-i2\pi\vec{K}'\cdot\vec{r})}{K_{z'}}dK_{x'}dK_{y'} \tag{5.1}$$

Here $\vec{K}'$ is the running vector, having wave components

$$K_{x'},\ K_{y'} \text{ and } K_{z'} = \sqrt{K^2 - K_{x'}^2 - K_{y'}^2}$$

The geometry is shown in Fig. 3. It is clear that the contribution of a given plane wave component $\exp(-i2\pi\vec{K}'\cdot\vec{r})$ is $1/K_{z'}$. Thus the induced wave amplitude corresponding to an incident spherical wave is

$$D_{0,h}^{spherical} = \frac{i}{4\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{K_{z'}}D_{0,h}^{plane}dK_{x'}dK_{y'} \tag{5.2}$$

where $D_{0,h}^{plane}$ are the amplitude of the forward-diffracted and diffracted waves induced in a perfect crystal by an incident plane wave with wave vector $\vec{K}'$, and have forms given in

Eq. (2.9) (assume the point source is located at the sample surface). The integration over $K_{y'}$ can be performed using stationary phase method (see Appendix A) and taken out,

$$\int_{-\infty}^{\infty} \frac{\exp[-i2\pi\sqrt{K^2 - K_{x'}^2 - K_{y'}^2}z']}{\sqrt{K^2 - K_{x'}^2 - K_{y'}^2}} dK_{y'} \approx \frac{\exp(-i2\pi K_{z'}z' + i\pi/4)}{\sqrt{K_{z'}z'}}; \text{ with } K_{z'} = \sqrt{K^2 - K_{x'}^2}$$

By noticing $K_{x'} = K\eta_0$ and $K_{z'} \approx K$, the forward-diffracted and diffracted waves caused by a point source are

$$D_0^{spherical} = A_0 \int_{-\infty}^{\infty} K \exp[i2\pi K\eta_0 x \sin\theta_B] Y(z) d\eta_0 \tag{5.3a}$$

$$D_h^{spherical} = A_h \int_{-\infty}^{\infty} K \exp[i2\pi K\eta_0 x \sin\theta_B] X(z) Y(z) d\eta_0 \tag{5.3b}$$

with $A_0 = \dfrac{i}{4\pi\sqrt{Kz'}} \exp[-i2\pi(\vec{K}_B \cdot \vec{r} - K\eta' \cos\theta_B z - 1/8)]$, $A_h = A_0 \exp(-i2\pi\vec{h}' \cdot \vec{r})$

and $\vec{K}_B = K(\cos\theta_B, \sin\theta_B)$.

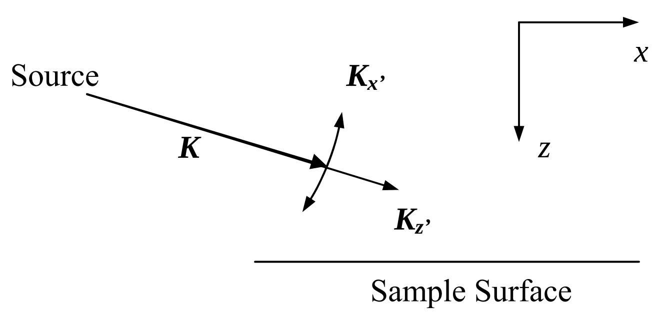

Fig. 3. Geometrical representation of a spherical wave incident on a single crystal.

Pre-factors A_0 and A_h are of no importance in describing the waves and will be dropped in following discussion. Eqs. (5.3a) and (5.3b) have the form of the Fourier transform, which maps the solution in reciprocal space to real space. Using plane-wave solution for diffraction on a crystal with uniform strain gradients given in Eqs. (9a) and (9b), we are able to obtain spatial distribution of the forward-diffracted and diffracted waves from Eqs. (5.3a) and (5.3b) caused by a point source:

$$D_0^{spherical} = K\int_{-\infty}^{\infty} \exp[i2\pi K\eta_0 x\sin\theta_B]\frac{\exp(-q^2/2)H_b(q)}{\exp(-q_0^2/2)H_b(q_0)}d\eta_0 \qquad (5.4a)$$

$$D_h^{spherical} = -K\sqrt{2b}\frac{\chi_h}{\sqrt{\chi_h\chi_{\bar{h}}}}\int_{-\infty}^{\infty} \exp[i2\pi K\eta_0 x\sin\theta_B]\frac{\exp(-q^2/2)H_{b-1}(q)}{\exp(-q_0^2/2)H_b(q_0)}d\eta_0 \qquad (5.4b)$$

These two equations can be valuated by numerical integration. For the purpose of analytical analysis, however, approximate equations would be useful. These are derived in the following.

b) Approximate Equations for Surface Intensity Distribution

For this purpose we use the asymptotic expansion of the analytical solution for an absorption crystal from Olver's theorem (Slater, 1960) (see Appendix B). The techniques used are very similar to those in ref. (Chukhovskii & Malgrange, 1989), but here we take absorption into account. In summary, we can expand a Hermite function into:

$$\begin{aligned}&\exp(-\frac{q^2}{2})H_b(q)\\ &\approx (t^2-1)^{-1/4}\{c_1\exp[-4\kappa\varsigma(t)]\times[1+O(\frac{1}{4\kappa})^{-1}]+c_2\exp[4\kappa\varsigma(t)][1+O(\frac{1}{4\kappa})^{-1}]\}, \qquad (5.5)\\ &\approx (t^2-1)^{-1/4}\{c_1w_1[\varsigma(t)]+c_2w_2[\varsigma(t)]\}\end{aligned}$$

where $\kappa = b/2 + 1/4$. Here the definitions of c_1, c_2, t and ς depend on the phase of q.

In case $|\arg(q)| < \pi/2$,

$$c_1 = \frac{e^{-\kappa}}{\sqrt{2}}(4\kappa)^{\kappa-1/4},\ c_2 = 0,\ t = \frac{q}{\sqrt{4\kappa}} \text{ and } \varsigma = \frac{1}{2}[t\sqrt{t^2-1} - \ln(t+\sqrt{t^2-1})].$$

In case $|\arg(q)| > \pi/2$,

$$c_1 = \frac{e^{-\kappa-\varepsilon b\pi i}}{\sqrt{2}}(4\kappa)^{\kappa-1/4}, \qquad c_2 = \frac{\sqrt{\pi}}{\Gamma(-b)\sqrt{2}}e^{\kappa}\kappa^{-\kappa-1/4}, \qquad t = -\frac{q}{\sqrt{4\kappa}} \qquad \text{and}$$

$$\varsigma = \frac{1}{2}[t\sqrt{t^2-1} - \ln(t+\sqrt{t^2-1})],$$

where $\varepsilon = -1$ if $\pi/2 < \arg(q) < \pi$ (negative strain gradient) and $\varepsilon = 1$ if $-\pi < \arg(q) < -\pi/2$ (positive strain gradient). Here we reuse symbol t, which does not represent sample thickness anymore. The asymptotic expansion of $\exp(-q^2/2)H_{b-1}(q)$ is obtained by using the recurrence relation of Hermite function:

$$\frac{\partial H_b(q)}{\partial q} = 2bH_{b-1}(q).$$

Differentiating both sides of Eq. (5.5) and arranging terms, one can obtain

$$e^{-\frac{q^2}{2}}H_{b-1}(q) \approx \frac{1}{2b}\begin{cases} -(t^2-1)^{-1/4}\{f_1(t)c_1w_1 + f_2(t)c_2w_2\}, & |\arg(q)| < \pi/2, t = q/\sqrt{4\kappa} \\ (t^2-1)^{-1/4} f_1(t)c_1w_1 & |\arg(q)| > \pi/2, t = -q/\sqrt{4\kappa} \end{cases} \quad (5.6)$$

where

$$f_1(t) = \sqrt{4\kappa}t - \sqrt{4\kappa(t^2-1)} - \frac{1}{2}\frac{t}{\sqrt{4\kappa}(t^2-1)},\ f_2(t) = \sqrt{4\kappa}t + \sqrt{4\kappa(t^2-1)} - \frac{1}{2}\frac{t}{\sqrt{4\kappa}(t^2-1)}.$$

The function w_1 represents a wave with amplitude decreasing with depth z, while function w_2 represents a wave with amplitude increasing with depth z. It is possible to calculate higher order terms from Olver's theorem and obtain expressions for higher order mirage peaks similar to those in ref. (Chukhovskii & Malgrange, 1989). When high order terms are considered, the interference fringes caused by rays emerging on the same position can be discussed. If we consider a normalized incident plane wave which has unit amplitude at the entry surface, when the deviation angle at the entrance surface η_0 has big negative value for a positive strain gradient or big positive value for a negative strain gradient so that $|\arg(q)| > \pi/2$, from Eqs. (5.4b), (5.5) and (5.6), the diffracted wave amplitude can be written as (neglecting high order terms):

$$X(q)Y(q) = -\sqrt{2b}\frac{\chi_h}{\sqrt{\chi_h\chi_{\bar{h}}}}\frac{\exp(-q^2/2)H_{b-1}(q)}{\exp(-q_0^2/2)H_b(q_0)} \approx W_1 + W_2,$$

$$W_1 = \frac{\chi_h}{\sqrt{\chi_h\chi_{\bar{h}}}}\frac{f_1(t)}{\sqrt{2b}}\exp[-4\kappa\varsigma(t) + 4\kappa\varsigma(t_0)], \quad (5.7a)$$

$$W_2 = \frac{\chi_h}{\sqrt{\chi_h\chi_{\bar{h}}}}\frac{f_2(t)c_2}{\sqrt{2b}c_1}\exp[4\kappa\varsigma(t) + 4\kappa\varsigma(t_0)], \quad (5.7b)$$

where t_0 is the value of t at the entrance surface, $t_0 = t(0)$. Below depth z_e at which $q(z_e) \sim 0$, or when η_0 has big positive value for a positive strain gradient (big negative value for a negative strain gradient) so that $|\arg(q)| < \pi/2$, $c_2 = 0$ and only wave 1 exists.

Consequently, the problem of x-ray Bragg diffraction from a crystal with a constant strain gradient illuminated with an incident spherical wave is reduced to evaluating two integrals,

$$D_{h1} = \int_{-\infty}^{\infty} K\exp[i2\pi K\eta_0 x\sin\theta_B]W_1 d\eta_0 \quad (5.8a)$$

$$D_{h2} = \int_{-\infty}^{\infty} K \exp[i2\pi K\eta_0 x \sin\theta_B] W_2 d\eta_0 \qquad (5.8b)$$

Here D_{h1} originates from the entrance surface, while D_{h2} originates from a layer beneath the sample surface. Equations (5.8-a,b) can be integrated by means of the stationary phase method (Appendix A). In the following discussion we assume a positive strain gradient. Let us write

$$W_1 = \frac{f_1(t)}{\sqrt{2b}} \frac{\chi_h}{\sqrt{\chi_h \chi_{\bar{h}}}} \exp[-4\kappa\varsigma(t) + 4\kappa\varsigma(t_0)] = \frac{\chi_h}{\sqrt{\chi_h \chi_{\bar{h}}}} F_1(t) \exp[-is(t) + is(t_0)],$$

$$W_2 = \frac{f_2(t)c_2}{\sqrt{2b}c_1} \frac{\chi_h}{\sqrt{\chi_h \chi_{\bar{h}}}} \exp[4\kappa\varsigma(t) + 4\kappa\varsigma(t_0)] = \frac{\chi_h}{\sqrt{\chi_h \chi_{\bar{h}}}} F_2(t) \exp[is(t) + is(t_0)],$$

where $s = \mathrm{Im}[4\kappa\varsigma(t)]$ and

$$F_1(t) = \frac{f_1(t)}{\sqrt{2b}} \exp\{\mathrm{Re}[-4\kappa\varsigma(t)] + \mathrm{Re}[4\kappa\varsigma(t_0)]\}$$
$$F_2(t) = \frac{f_2(t)c_2}{\sqrt{2b}c_1} \exp\{\mathrm{Re}[4\kappa\varsigma(t)] + \mathrm{Re}[4\kappa\varsigma(t_0)]\}.$$

Defining the phase terms S_1, S_2 in Eqts. (5.4):

$$S_1 = 2\pi K\eta_0 x \sin\theta_B - s(t) + s(t_0),$$

$$S_2 = 2\pi K\eta_0 x \sin\theta_B + s(t) + s(t_0).$$

For the phase to be stationary, we need to find the point at which $\partial S_j / \partial\eta_0 = 0$. The derivative of s with respective to η_0 can be obtained from,

$$\frac{\partial}{\partial\eta_0}(4\kappa\varsigma) = \frac{\partial}{\partial t}(4\kappa\varsigma)\frac{\partial t}{\partial\eta_0} = 4\kappa\sqrt{t^2 - 1}\frac{\partial t}{\partial\eta_0}.$$

For a crystal with absorption, both χ_{0i} and χ_{hi} are not zero. In the case $\sigma_0 = \left|\frac{\chi_{0i}}{\chi_{hr}}\right| << 1$, $\left|\frac{\chi_{hi}}{\chi_{hr}}\right| << 1$ and $\sigma_h = \left|\frac{\chi_{hi}}{\chi_{hr}}\right| \cos\upsilon_h$ (υ_h is the phase difference between χ_{hr} and χ_{hi}, equal to 0 or π for centro-symmetric structures), following approximations can be made

$|b| \approx \left|\frac{2a\chi_{hr}^2}{\nu'}\right|$, $b \approx i|b|(1+2i\sigma_h)$,

$$\frac{\partial}{\partial\eta_0}(4\kappa\varsigma) \approx \pm\frac{2\sin 2\theta_B}{|\chi_{hr}|}|b|(i\sqrt{\nu_r^2-1} + \frac{\nu_r\sigma_0 + \sigma_h - 1/4|b|}{\sqrt{\nu_r^2-1}}),$$

with $\nu_r = \frac{\eta(z)\sin 2\theta_B + \chi_{0r}}{|\chi_{hr}|} = \nu_{r0} + \nu_r' z$, $\frac{\partial\nu_r}{\partial\eta_0} = \frac{\sin 2\theta_B}{|\chi_{hr}|}$ and "+" if $\nu_r > 1$; "-" if $\nu_r < -1$.

This approximation is not valid when $|\nu_r|$ is very close to 1, but works well when $\nu_r^2 - 1 > 1$. Thus, $\frac{\partial s}{\partial\eta_0} = \pm\frac{2\sin 2\theta_B}{|\chi_{hr}|}|b|\sqrt{\nu_r^2-1}$.

The condition for the phase to be stationary imposes restriction on the travel path of the x-ray. When $\nu_r < -1$, for wave 1,

$$\frac{\partial S_1}{\partial\eta_0} = 0 \Rightarrow 2\pi Kx\sin\theta_B + \frac{2\sin 2\theta_B}{|\chi_{hr}|}|b|(\sqrt{\nu_r^2-1} - \sqrt{\nu_{r0}^2-1}) = 0 \quad (5.9a)$$

Similarly, for wave 2:

$$\frac{\partial S_2}{\partial\eta_0} = 0 \Rightarrow 2\pi Kx\sin\theta_B - \frac{2\sin 2\theta_B}{|\chi_{hr}|}|b|(\sqrt{\nu_r^2-1} + \sqrt{\nu_{r0}^2-1}) = 0 \quad (5.9b)$$

When $\nu_r > 1$, wave 2 does not exist since $c_2 = 0$, and for wave 1,

$$2\pi Kx\sin\theta_B - \frac{2\sin 2\theta_B}{|\chi_{hr}|}|b|(\sqrt{\nu_r^2-1} - \sqrt{\nu_{r0}^2-1}) = 0 \quad (5.9c)$$

Eqts. (5.9-a, b, c) are the ray trajectory functions that describe the travel path of the reflected wave in a crystal with a constant strain gradient. They can be also obtained from optical theory of dynamical diffraction (Gronkowski & Malgrange, 1984).

The second part of the problem is determining the reflection intensity distribution at the sample surface ($z = 0$) as a function of x. For D_{h1}, the phase is not stationary at the surface, but the integral can be performed exactly. In the symmetric Bragg case the reflection intensity distribution of wave 1 at the sample surface has the form:

$$I_1 = \left|D_{h1}\right|^2 = \exp(-\frac{\mu_0 x}{\cos\theta_B})[\frac{J_1(\frac{x\tan\theta_B}{2\xi_e})}{x\sin\theta_B}]^2 . \tag{5.10}$$

I_1 has a maximum value at $x = 0$, which is equal to $\rho_1 = (4\xi_e \cos\theta_B)^{-2}$. The first zero point of I_1 is located at $x = 7.66\xi_e / \tan\theta_B$. From the property of Bessel function, most intensity of the first wave falls within the range from zero to its first zero point. If we normalize $I_1(0)$ to unity, the form of I_1 here is identical to Eqt. (4) in our paper, which describes the surface reflection intensity distribution for a semi-infinite strain free crystal.

An approximate expression for D_{h2} can also be derived using stationary-phase method. For a positive strain gradient, when $\nu_r < -1$ the second wave field is excited, and approximately,

$$f_2(t) \approx (1+i)\sqrt{|b|}(\sqrt{\nu_r^2 - 1} - \nu_r)(1 + i\frac{\sigma_0}{\sqrt{\nu_r^2 - 1}}),$$

$$\mathrm{Re}(4\kappa\varsigma) \approx -|b|[2\sqrt{\nu_r^2-1}\sigma_0 + \frac{\nu_r(\sigma_h - 1/4|b|)}{\sqrt{\nu_r^2-1}}] - (1/2 - 2|b|\sigma_h)\ln(\sqrt{\nu_r^2-1} - \nu_r) + P,$$

with $P = \mathrm{Re}[-2\kappa \ln \frac{(1+i)\sqrt{|b|}}{\sqrt{4\kappa}}]$.

At $z = 0$ for the phase to be stationary, it requires

$$\sqrt{\nu_{r0}^2 - 1} = \frac{\pi K |\chi_{hr}|}{4|b|\cos\theta_B} x = u$$

The second derivative of $s(t_0)$ with respect to η_0 can be derived from,

$$\frac{\partial^2}{\partial\eta_0^2}\mathrm{Im}[4\kappa\varsigma(t_0)] = \frac{2\sin^2 2\theta_B |b|}{|\chi_{hr}|^2}\frac{\nu_{r0}}{\sqrt{\nu_{r0}^2-1}} = -\frac{2\sin^2 2\theta_B |b|}{|\chi_{hr}|^2}\frac{\sqrt{u^2+1}}{u}.$$

Therefore, we arrive at

$$D_{h2} \approx \frac{\chi_h}{\sqrt{\chi_h \chi_{\bar{h}}}} \frac{c_2}{c_1} \frac{\sqrt{i\pi} K |\chi_{hr}|}{\sqrt{2b}\sin 2\theta_B} (u + \sqrt{u^2+1})^{4|b|\sigma_h} (\frac{u}{\sqrt{u^2+1}})^{1/2}$$
$$\times \exp\{-2|b|[2u\sigma_0 - \frac{\sqrt{u^2+1}}{u}(\sigma_h - 1/4|b|)] + 2P\} \exp\{i[S_2(u) - \frac{\pi}{4}]\}.$$

For the intensity, one obtains

$$I_2 \approx \rho_2 (u + \sqrt{u^2+1})^{8|b|\sigma_h} (\frac{u}{\sqrt{u^2+1}}) \exp(1 - \frac{\sqrt{u^2+1}}{u}) \exp[-4|b|(2u\sigma_0 - \frac{\sqrt{u^2+1}}{u}\sigma_h)] \quad (5.11)$$

with $\rho_2 \approx \frac{K^2 |\chi_{hr}|^2 \pi^2}{\sin^2 2\theta_B} \frac{\exp(-\pi|b| - 4|b|\sigma_h)|b|^{4|b|\sigma_h}}{|b|^2 |\Gamma(-b)|^2} \approx \rho_1 \frac{\exp(-\pi|b| - 4|b|\sigma_h)|b|^{4|b|\sigma_h}}{|b|^2 |\Gamma(-b)|^2}$.

We notice $\exp(-8|b|u\sigma_0)$ is the linear kinematical absorption, since

$$\exp(-8|b|u\sigma_0) = \exp(-2\pi K |\chi_{0i}| x/\cos\theta_B) = \exp(-\mu_0 x/\cos\theta_B).$$

Other terms in Eq. (5.11) are due to dynamical diffraction. When $u >> 1$ or equivalently $\sqrt{\nu_{r0}^2 - 1} >> 1$, the following approximation is valid,

$$\frac{u}{\sqrt{u^2+1}} \approx \frac{\sqrt{u^2+1}}{u} \approx 1,$$

and Eqt. (5.11) turns into,

$$I_2 \approx \rho_2 \exp(4|b|\sigma_h) \exp\{-8|b|u\sigma_0[1-(1/u)(\sigma_h/\sigma_0)\ln(u+\sqrt{u^2+1})]\}, \quad (5.12)$$

which is similar to Eqt. (2), and is only applicable for x not close to zero ($|\nu_{r0}| >> 1$). If the crystal is perfect then $|b| \to \infty$, thus $\rho_2 = 0$ and the second wave does not exist. The intensity of wave 1 is described by Eqt. (5.10), which is identical to Eqt. (4) in our paper. For a transparent crystal that has $\sigma_0 = \sigma_h = 0$, b is a pure imaginary number and

$$|\Gamma(-b)|^{-2} = \frac{|b|\sinh(\pi|b|)}{\pi}.$$

Consequently, Eqt. (5.11) is reduced to

$$I_2 \approx \rho_1 \frac{1-\exp(-2\pi|b|)}{2\pi|b|} u(u^2+1)^{-1/2} \exp(1-\frac{\sqrt{u^2+1}}{u}), \quad (5.13)$$

which is equivalent to the equation obtained by Chukhovskii and Malgrange (Chukhovskii & Malgrange, 1989) for a transparent crystal, except that there is an additional (last) exponential term in our derivation. In kinematical limit where the strain gradient becomes infinity so that $|b|$ becomes zero, I_2 turns into

$$I_2 = \rho_1 \exp(-\mu_0 x/\cos\theta_B), \quad (5.14)$$

which is the equation predicted by the kinematical theory.

Appendix A

For an integral of the type

$$I = \int_{-\infty}^{\infty} F(x) \exp[iS(x)] dx, \qquad \text{(A1)}$$

the phase $S(x)$ is generally large and rapidly varying. The integration over most of this range would be averaged to almost zero because of the rapid oscillation of $\exp(iS)$, except in the neighborhood of a saddle point x_0 where the phase is stationary. In other words, the first derivative of $S(x)$ is zero at x_0. The integral therefore can be evaluated only around x_0. If we may expand S as a Taylor series around this point,

$$S(x) = S(x_0) + \frac{1}{2} S''(x_0)(x - x_0)^2 + \cdots \qquad \text{(A2)}$$

and $F(x)$ is a slowly varying function around x_0, an approximate value of the integral can be obtained

$$\begin{aligned} I &\approx \int_{-\infty}^{+\infty} F(x_0) \exp[iS(x_0) + i\frac{1}{2} S''(x_0)(x - x_0)^2] dx \\ &= F(x_0) \exp[iS(x_0)] \int_{-\infty}^{+\infty} \exp[i\frac{1}{2} S''(x_0)(x - x_0)^2] dx \qquad \text{(A3)} \\ &= F(x_0) \sqrt{\frac{2\pi}{|S''(x_0)|}} \exp\{[iS(x_0) \pm \frac{\pi}{4}]\} \end{aligned}$$

where "+" sign is taken if $S''(x_0) > 0$ and "-" sign is taken when $S''(x_0) < 0$.

Appendix B

Olver (Slater, 1960) discussed the asymptotic expansions of solutions to equation that has the form

$$\frac{d^2w}{dz^2} = [k^2 z^n + f(z)]w$$

He showed that for $n = 0, \pm 1$ and large values of *k*, asymptotic expansions of the solutions can be obtained in three cases. Here we will consider only the first case, $n = 0$, where the equation becomes :

$$\frac{d^2w}{dz^2} = [k^2 + f(z)]w \tag{B1}$$

Equation (B1) has two independent asymptotic solutions

$$\begin{aligned} w_1(z) &= e^{-kz}\{\sum_{s=0}^{M-1} \frac{(-1)^s A_s(z)}{k^s} + O(k^{-M})\} \\ w_2(z) &= e^{kz}\{\sum_{s=0}^{M-1} \frac{A_s(z)}{k^s} + O(k^{-M})\} \end{aligned} \tag{B2}$$

where $A_0(z) = 1, A_{s+1}(z) = -\frac{1}{2}A_s'(z) + \frac{1}{2}\int f(z)A_s(z)dz + K_s$, and K_s is an arbitrary constant.

If we define $t = q/\sqrt{4\kappa}$, Eqt. 4-c becomes:

$$Y''(t) = (4\kappa)^2(t^2 - 1)Y(t) \tag{B3}$$

Furthermore, we consider the transformation $\varsigma = \frac{1}{2}\{t\sqrt{t^2 - 1} - \ln(t + \sqrt{t^2 - 1})\}$. The square root and logarithm are both many-value functions. We chose the principal branch for the many-value function logarithm ($|\arg| < \pi$) and the branch with positive real component for the many-value function square-root, so $\left|\arg(t)\right| < \pi/2$. A cut line is set from 1 to -∞ along the real axis on t plane. By putting

$$w = (\frac{dt}{d\varsigma})^{-\frac{1}{2}} Y(t) = (t^2-1)^{1/4} Y(t) \tag{B4}$$

we have

$$\frac{d^2 w[\varsigma(t)]}{d\varsigma^2} = \{(4\kappa)^2 + f[\varsigma(t)]\} w[\varsigma(t)] \tag{B5}$$

where $f[\varsigma(t)] = \frac{1}{2(t^2-1)^2} - \frac{5t^2}{4(t^2-1)^3}$.

The solution of Eqt. B5 is given by the linear combination of w_1 and w_2,

$$\begin{aligned} w(\varsigma) &= c_1 w_1(\varsigma) + c_2 w_2(\varsigma) \\ w_1(\varsigma) &= e^{-4\kappa\varsigma}\{\sum_{s=0}^{M-1} \frac{(-1)^s A_s(\varsigma)}{(4\kappa)^s} + O[(4\kappa)^{-M}]\} \approx e^{-4\kappa\varsigma}\{1 + O[(4\kappa)^{-1}]\} \\ w_2(\varsigma) &= e^{4\kappa\varsigma}\{\sum_{s=0}^{M-1} \frac{A_s(\varsigma)}{(4\kappa)^s} + O[(4\kappa)^{-M}]\} \approx e^{4\kappa\varsigma}\{1 + O[(4\kappa)^{-1}]\} \end{aligned} \tag{B6}$$

We should note that the above asymptotic expansion is limited to $\left|\arg(q/\sqrt{4|\kappa|})\right| < \pi/2$, but can be extended to $\left|\arg(q/\sqrt{4|\kappa|})\right| > \pi/2$ by replacing q with $Q = -q$. If we define $t = Q/\sqrt{4\kappa}$, the form of Eq. (B3) does not change but now $\left|\arg(Q/\sqrt{4|\kappa|})\right| < \pi/2$ and all results are the same.

The coefficients c_1 and c_2 can be determined from the comparison of leading terms with the known asymptotic expansion of $Y(q)$ as $|q| \to \infty$. In case $\left|\arg(q)\right| < \pi/2$ and $|q| \to \infty$,

$$\exp(-q^2/2) H_b(q) \sim \exp(-q^2/2)(2q)^b = \exp(-2\kappa t^2)(16\kappa t^2)^{\kappa-1/4},$$

and

$$w_1 \sim \exp[-2\kappa(t^2 - 1/2)](4t^2)^{\kappa},$$

$$w_2 \sim \exp[2\kappa(t^2 - 1/2)](4t^2)^{-\kappa},$$

$$(t^2 - 1)^{-1/4} \sim (t^2)^{-1/4}.$$

From the comparison of the leading terms, one obtains,

$$c_1 = e^{-\kappa}(4\kappa)^{\kappa - 1/4}/\sqrt{2},$$
$$c_2 = 0.$$

In the case $|\arg(q)| > \pi/2$ so $|\arg(-q)| < \pi/2$, $t = -q/\sqrt{4\kappa} = Q/\sqrt{4\kappa}$,

$$\exp(-q^2/2)H_b(q) \sim e^{\frac{Q^2}{2}} \frac{\sqrt{\pi}}{\Gamma(-b)} Q^{-b-1} + e^{-\frac{Q^2}{2}} (2Q)^b e^{-\varepsilon b\pi i}$$
$$= \frac{\sqrt{\pi}}{\Gamma(-b)} (4\kappa t^2)^{-\kappa - 1/4} \exp(2\kappa t^2) + 2^{2\kappa - 1/2} (4\kappa t^2)^{\kappa - 1/4} \exp(-\varepsilon b\pi i) \exp(-2\kappa t^2).$$

Therefore,

$$c_1 = e^{-\kappa}(4\kappa)^{\kappa - 1/4} \exp(-\varepsilon b\pi i)/\sqrt{2}, \quad \varepsilon = 1 \text{ if } \arg(Q) > 0; \ \varepsilon = -1 \text{ if } \arg(Q) < 0.$$

$$c_2 = \frac{\sqrt{\pi}}{\Gamma(-b)\sqrt{2}} e^{\kappa} \kappa^{-\kappa - 1/4}.$$

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