Computer simulation of bent perfect crystal diffraction profiles

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ABSTRACT
Various theoretical methods for calculating diffraction profiles of perfect crystals are available in literature. Although these methods hold within certain validity ranges due to their inherent approximations, they constitute the current state-of-the-art of numerical computation of diffraction profiles.

In this paper we summarize the theory of Zachariasen for flat crystals, the multi-lamellar approximation for bent crystals and the Penning-Polder approximation for bent Laue crystals. Some examples of their results are presented. Another method to calculate the diffraction profile consists in solving the Takagi-Taupin equations. The finite difference method, that provides a numerical solution of these equations, is briefly discussed.

A new method for solving numerically these equations using the finite element method is proposed. This method is very flexible, because it can consider a crystal with an arbitrary shape and cover the case of critical regions (i.e., inhomogeneities and deformations) with fine elements. In addition, it can couple naturally the diffraction calculation with thermal or mechanical crystal deformations. These deformations are generally induced by the x-ray beam (heat load), the crystal bender (mechanical stress) or are intrinsic to the crystal (inhomogeneities, impurities, dislocations, etc.). An example of the feasibility of this method is shown.

Keywords: crystal optics, dynamical diffraction, bent or distorted crystals, perfect crystals, finite element method, finite difference method, Takagi-Taupin equations

1. INTRODUCTION

The diffraction profile of a perfect crystal is the intensity response of such a crystal as a function of the rocking angle when a collimated monochromatic incident photon beam impinges on the crystal. The dynamical diffraction theory is used to calculate the diffraction profiles of parallel, plane, and unstrained slabs of perfect crystals. When the crystal itself is deformed, either locally or over the whole crystal volume, the standard dynamical theory fails to predict the diffraction profile correctly. The most usual case of crystal deformation is a curvature. Other lattice deformations are caused by local inhomogeneities or inclusions, thermal gradients between the crystal surfaces, errors in surface cutting and polishing, crystal mosaicity, etc. Any crystal deformation may affect the diffraction profile when it creates a sufficiently large change in the parallelism of the Bragg planes contributing to diffraction. In the case of a deformation produced by a cylindrical bending, there are approximate methods (multi-lamellar and Penning-Polder) that give reasonable results provided they are used within their validity ranges. They cannot be applied in all real cases because the experimental conditions do not meet their applicability constraints.

In order to calculate the diffraction profile for a general deformation, one has to calculate the amplitude of the electric field inside the crystal. This is done by solving directly the Takagi-Taupin (TT) equations which are obtained from the Maxwell equations in a deformed periodic medium such as a crystal. The TT equations consist in a system of hyperbolic partial derivative equations. The problem of determining the diffracted beam by a crystal reduces to solving these equations with appropriate boundary conditions (the crystal volume itself, the deformation field in the crystal, and the incident x-ray field). Analytical solutions can be found only for some special cases with simple crystal geometries and with simplified models of the crystal strength and imperfections. Numerical methods seem to be more adequate in realistic cases, where the boundary conditions are modeled or inferred from measurements. Several numerical models for solve the TT equations have been proposed, and most of them are based on the finite

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difference method. None of them can solve the general problem with any given crystal geometry and a realistic map of the crystal imperfections.

Our aim is to provide a software package that permits to solve numerically the TT equations under nearly any condition. We have already implemented a computer code to calculate diffraction profiles with the finite difference method (FDM). Moreover, we propose a novel and more general method for solving the TT equations: The finite element method (FEM).

The FDM code is being used to validate the FEM code under development, and to identify the limitations of the FDM in comparison with the FEM. It is based on existing codes used for X-ray topography, which have been enhanced to calculate diffraction profiles.

The FEM not only provides a procedure to solve the TT equations (it is, in fact, a general method to solve numerically partial derivative equations), but also allows to couple in a natural way the calculation of the X-ray propagation with both the mechanical deformation and the thermal load of the crystal. The calculated diffraction profiles can be used by other computer codes that simulate the behavior of a whole synchrotron beamline, such as ray-tracing codes and phase-space analysis programs. An application example is the calculation of the diffraction of a synchrotron beam by a crystal mounted in a bender. The FEM allows to compute at a time the mechanical deformation created by the bender in the crystal, the thermal strain originated by the beam and the diffraction properties of the crystal. Another important application field is X-ray topography. The quantitative analysis of an experimental X-ray topograph is done by comparing it with ab-initio calculations (solving the TT equations with a model of the crystal deformation).

2. FLAT CRYSTALS

The foundations of the dynamical theory were put by Darwin.\textsuperscript{1,2} He considered multiple reflection between atomic planes in a perfect crystal, which produce constructive and destructive interferences in the reflected beams. The diffracted beam is calculated by adding the individual beams reflected by each atomic plane. A modern textbook describing this model can be found in Ref. 3.

A more rigorous theory was introduced later by Ewald.\textsuperscript{4,5} The crystal is considered as a periodic net of dipoles excited by the incident radiation. The electromagnetic radiation waves produced by these dipoles interfere to form the diffracted beam. Laue\textsuperscript{6} reformulated this theory by solving the Maxwell equations in a medium with a periodic dielectric constant. Basic references to the Ewald-Laue theory can be found in the paper of Batterman and Cole\textsuperscript{7} (B&C) and in the book of Zachariasen.\textsuperscript{8} Although the B&C paper is physically more intuitive, it is preferred to formulate the equations following Zachariasen, because their form is more compact and their numerical implementation is easier.

The diffraction profile of a single perfect parallel-sided crystal of thickness \( t \) in Bragg (or reflection) geometry can be calculated as:

\[
R_{\text{bragg}}(\Delta) \equiv \frac{1}{|b|} \frac{I_H}{I_0} = \frac{1}{|b|} \left| \frac{x_1 x_2 (c_1 - c_2)}{c_2 x_1 - c_1 x_2} \right|^2.
\]  

For Laue (or transmission) geometry we have:

\[
R_{\text{laue}}(\Delta) \equiv \frac{1}{|b|} \frac{I_H}{I_0} = \frac{1}{|b|} \left| \frac{x_1 x_2 (c_1 - c_2)}{x_2 - x_1} \right|^2,
\]

where \( \Delta = \theta - \theta_H \), \( \theta \) is the incidence angle, \( \theta_H \) is the kinematical Bragg angle, \( I_H \) is the intensity of the external diffracted wave, \( I_0 \) is the intensity of the incident wave, \( c_1 = \exp(-i\phi_1 t), c_2 = \exp(-i\phi_2 t), \phi_1 = 2\pi k_0^2 / q_0, \phi_2 = 2\pi k_0^2 / \gamma_0, \gamma_0 (\gamma_H) \) is the direction cosine of the incident (diffracted) wave and the other quantities are defined as:

\[
\left( \begin{array}{c}
\delta_0 \\
\delta_0^\prime
\end{array} \right) = \frac{1}{2} \left( \Psi_0 - z \pm \sqrt{qP^2 + z^2} \right),
\]

\[
\left( \begin{array}{c}
x_1 \\
x_2
\end{array} \right) = \frac{-z \pm \sqrt{qP^2 + z^2}}{P\Psi_H},
\]
\[ z = \frac{1 - b}{2} \Psi_0 + \frac{b}{2} \tau, \]

\( q = b\Psi_H \Psi_B, \tau \simeq 2\Delta \sin(2\theta_B), P \) is the polarization factor, \( \Psi_H \) is the Fourier component of the electrical susceptibility \( \Psi_0, b = \gamma_0/\gamma_h \) is the asymmetry factor, \( k = 1/\lambda \) is the wavevector in vacuum and \( \lambda \) is the wavelength. The above formulation is coded in the XCRYSTAL computer program that is available in the XOP package. Note that the above expression for \( \tau \) is valid only for Bragg angles far from \( \theta_B = 90^\circ \), that is, it does not hold for normal incidence. However, the exact value for \( \tau \) given by Eq. (3.144b) in Ref. 8 is coded in XCRYSTAL. This guarantees that accurate results are also obtained for the normal incidence case. The diffraction curves for flat crystals presented in this paper are computed with this code.

3. BENT CRYSTAL: APPROXIMATE METHODS

When a perfect crystal is elastically bent, the diffracted beam is modified with respect to the plane case because of two reasons. The first is the bent geometry, which generates an angular distribution of the entrance angle of the rays with respect to the crystal surface along the beam footprint. This angular distribution causes changes in the total diffracted intensity. As we are not interested in this effect, that can be easily treated by any ray-tracing program, we will always consider collimated beams with a cross section small enough to produce a negligible angular dispersion on the bent crystal surface. The second reason is that, when the crystal curvature radius is "small enough", the crystallographic atomic planes suffer a distortion and the local reflectivity of the crystal at any point of its surface varies drastically. In other words, the mechanical tensions related to the bending entail a misalignment between the atomic planes causing, in general, an enlargement of the diffraction profiles.

Two approximate methods are proposed to calculate the crystal diffraction profiles for bent crystals: the multi-lamellar (ML) method and the Penning-Polder (PP) method. The latter is only applicable for crystals in transmission geometry. Both are discussed in this section.

These methods are based on the dynamical diffraction theory, and their validity is restricted to slightly distorted crystals. The curvature increases the diffraction profile width and decreases the peak height. When the crystal is bent strongly, the kinematical theory applies. A criterion to characterize the dynamical-to-kinematical transition can be found in Ref. 10.

3.1. The multi-lamellar method

The main idea behind this method is to decompose the crystal (in the direction of beam penetration) in several layers of a suitable thickness. Each layer behaves as a perfect crystal, thus the diffracted and transmitted beams are calculated using the dynamical theory for plane crystals. The different layers are misaligned one with respect to the others in order to follow the cylindrical surface of the crystal plate. This model was first introduced by White\(^\text{11}\) and further developed by, among others, Egert and Dachs\(^\text{12}\) and Boeuf et al.\(^\text{13}\). It has been used by Suortti et al.\(^\text{14,15}\) for optimization of monochromators for inelastic scattering and coronary angiography applications. It has also been used by Caciuffo et al.\(^\text{16}\) for simulating crystal analyzers for fusion plasma diagnostics.

In the multi-lamellar method the angular parameter \( y \) (related to the deviation of the incident angle from the Bragg angle) is assumed to be a function of the depth from the crystal entrance surface for a fixed direction of the incident beam. At the entrance surface the \( y \) value is called \( y_0 \) and its value can be taken from Eq. (3.141) in Ref. 8:

\[ y_0 = \frac{z}{\sqrt{|b|P|\Psi_H|}} = \frac{1 + b \Psi_0 + \frac{b}{2} \tau}{\sqrt{|b|P|\Psi_H|}}, \]

where \( z, \tau \) and all the other parameters are the same as in Eq. 5. For a cylindrically bent crystal, with a curvature radius \( \rho \), and a depth \( t \), it holds: \( y = y_0 + cA \), where \( A \) is the reduced thickness defined as:

\[ A = \frac{\pi \rho|\Psi_H|}{\lambda \sin(\theta_B - \alpha) \sin(\theta_B + \alpha)} t, \]
where $\alpha$ is the asymmetry angle (defined as the angle between the diffraction planes and the crystal entrance surface). The parameter $c$ is a dimensionless quantity related to $\rho$ through:

$$c = \frac{\sin(\theta_B - \alpha)(b - 1)}{\pi|\Psi_H|^2 b \rho} \left[ 1 + b(1 + \nu) \sin^2(\theta_B + \alpha) \right],$$

where $\nu$ is the Poisson ratio of the used material. Each perfect crystal slab has a reduced thickness $\Delta A = 2/c$ and a misorientation $\Delta y = 2$ relative to the adjacent one. The total reflectivity of the given set of layers can be computed by writing the energy balance for the different layers, which leads, in the case of $n$ layers, to:

$$R = \sum_{j=1}^{n} r_j \left( \prod_{k=0}^{j-1} t_k \exp(-\mu S_k) \right),$$

where $S_k$ is the x-ray path inside the $k$-th layer, $\mu$ is the absorption coefficient of the crystal material, $r_j$ and $t_i$ are the reflectivity and transmission ratio for the $i$-th layer, respectively. The $r_j$ values in Eq. (9) are calculated using the Eqs. (1) and (2) for the Bragg and Laue cases, respectively. For $t_i$ the Eqs. (3.138) and (3.131) of Ref. 8 are used for the Bragg and Laue cases, respectively.

We have developed a computer code which makes use of the equations of the lamellar model for both Bragg and Laue crystals. This code evolved from the code used by Caciuffo et al.\textsuperscript{16} and has been integrated in the XCRYSTAL\_BENT module of XOP.

In the ML model it is assumed that the crystal is perfect inside a given lamella, thus the crystal curvature cannot be large, otherwise it would originate local strains in the crystalline planes. The model is valid for crystals sufficiently thick to guarantee the existence of several lamellae. The model fails if the crystal thickness is of the order of or smaller than the lamella thickness. This may occur in Laue cases, where the crystal should be thin enough to guarantee a high transmission. The oscillations found in Laue profiles calculated with the ML model are due to unphysical interferences between the crystal lamellae. A detailed description of the assumptions of this method is in Refs. 17 and 18 and a good validation with experiments is in the paper by Erola \textit{et al.}\textsuperscript{15}

![Figure 1. Left: multi-lamellar calculations for a 5 mm thick, symmetrical Si 111 crystal at 8 keV in Bragg geometry. The different curves (from wider to narrower) correspond to curvature radii of 10, 50, 100 and 500 cm, respectively. Note the convergence of the curves to the flat crystal case when the curvature is decreased. Right: Laue diffraction profiles computed with ML (continuous) and PP (dashed) models for a Si 111 crystal, $\alpha = 63.78^\circ$, $t = 0.7$ mm and $\rho = 13$ m. Notice the unphysical oscillations in the multi-lamellar mode, due to the algorithm characteristics.](image)

### 3.2. The Penning-Polder method

A computer code based on the model by Penning and Polder\textsuperscript{19} was developed and is available in the XCRYSTAL\_BENT module of XOP. In the ray-optical theory of Penning and Polder the x-ray beam in a distorted crystal
is assumed to be a pseudo-plane Bloch wave ("wavefield ray") propagating parallel to the local Poynting vector. The crystal is supposed to be composed of perfect crystal parts where the dynamical theory for undistorted crystals can be applied. The wavefield is preserved passing from one part of the crystal to the next. Diffraction phenomena (the interference between two wavefields) are neglected. Thus, the Pendellösung fringes are not simulated with this model.

Following this theory the equation of the trajectory of a x-ray beam in a bent crystal with constant strain gradient $\beta$ is found to be:

$$
\left[ \xi_i + \frac{1}{\xi_i} + \frac{2\beta z}{\tan \theta_B} \right]^2 - \left[ 2\beta z + \xi_i - \frac{1}{\xi_i} \right]^2 = 4,
$$

(10)

where $\xi_i$ is the amplitude ratio between the transmitted and diffracted plane wave components ($\xi_i = D_\lambda / D_0$) at the entrance face of the crystal. The subscript $i$ stands for incident surface whilst the subscript $e$ is found below, stands for exit surface. The crystal axes are defined as in Fig. 3.

One can easily recognize that Eq. (10) is a hyperbola, whereas in the ML model the beam trajectories are straight. This equation holds for both Bragg and Laue cases. Some problems arise, however, in the total reflection angle owing to the anomalous absorption effect predicted by the theory. Thus, the Penning-Polder method is only applicable to the Laue case.

From an incident beam with intensity $I_0$ two wavefields are generated inside the crystal. The relations between the intensity of the incident beam and those of the diffracted and transmitted beams are:

$$
I_{R_j} = I_0 \frac{\xi_{ej}^2}{\xi_{ej}^2 + b} \exp \left\{ -\frac{\mu t}{\cos(\theta_B - \chi)} \left[ 1 + \frac{b - 1}{2t\beta} (\xi_{ej} - \xi_{ij}) + \frac{P_e}{\beta} \ln \frac{\xi_{ej}}{\xi_{ij}} \right] \right\}; \quad I_{T_j} = \frac{b}{\xi_{ej}^2} I_{R_j},
$$

(11)

where $j$ designates the propagation mode index, $\epsilon = \text{Im}(\Psi_H) / \text{Im}(\Psi_0)$, and $\chi = (\pi/2) - \alpha$, and the other quantities have already been defined. The values $\xi_{ej}$ at the exit surface of the crystal are related to the corresponding values $\xi_{ij}$ through:

$$
\frac{1}{\xi_{ej}} - \frac{1}{\xi_{ij}} = \frac{1}{\xi_{ij}} - 2\beta z.
$$

(12)

The strain gradient $\beta$ for a cylindrically bent crystal is given by:

$$
\beta = \frac{b - 1}{P_0 \Psi_H} \left[ 1 + \left( \cos 2\theta_B + \cos 2\chi \right) \frac{(1 + \nu)}{2} \right].
$$

(13)

In Eq. (13) the crystal is assumed to be elastically isotropic. This approximation is also done in our program although it would be straightforward to allow for the elastic anisotropy of asymmetrically cut crystals as it was done, for instance, in Ref. 20 only for crystals with cubic lattices. We have not included this feature in our program, because after several comparison tests we stated that for most applications cases of practical interest the anisotropy produce minor effects in the broadening of the diffraction profile.

An important feature which was included in the program but does not appear in the original PP theory is that the wave packet is actually made up of four parts and not of two, as described above. Two of them can be denoted as normal wavefields, whereas the other two are the so-called "created wavefields". It was shown\textsuperscript{21} that the latter arise from the interbranch scattering of the dispersion surface. The intensity of the created wave fields amount to a fraction $\exp(-2\pi|\beta_e|/|\beta|)$ of the original wavefield, where $\beta_e$ is the critical strain gradient $\beta_e = \frac{4\rho}{\lambda}$, where $\lambda$ is the Pendellösung period for a symmetrically cut crystal. For the sake of simplicity the assumption is made that the intensity of the created wave fields does not affect the reflected beam.

The reflectivity profile of a bent symmetrical ($\alpha = 90^\circ$) crystal is equal to that of an unstrained crystal. The PP model holds only for crystals with weak deformations, i.e., the curvature radius $\rho$ fulfills the condition $\rho \gg 2\Lambda \sin \theta / |\Psi_H|$, where $\Lambda$ is the Pendellösung length.
Figure 2. Penning-Polder calculations for a Si 111 crystal at $E = 17479 \text{ eV}$, $t = 525 \text{ lm}$, $P = 1$, $\alpha = 55^\circ$ and different values of curvature radius: $p = 1.1$ (dashed), 3.6 (dotted) and 7.5m (continuous line). These simulations agree qualitatively with the experimental data by Erola et al.\textsuperscript{15}

4. BENT CRYSTALS: TAKAGI-TAUPIN EQUATIONS

The Takagi-Taupin equations\textsuperscript{22,23} describe the behavior of the electromagnetic field inside a crystal, and can be used to determine the diffracted and transmitted beams for a distorted crystal. The calculation of reflection profiles requires the solution of these equations. Analytical solutions have been found only for particular cases of the strain field in Laue\textsuperscript{22,24} and in Bragg\textsuperscript{25,26} geometries, using either the Riemann or the Green function methods. Several authors developed codes to solve numerically the TT equations, but most of them restricted their analyses to simple cases of curvature and/or deformation, like cylindrical bending. We have chosen to use and solve the general form of the TT equations in order to provide, for future applications, a general frame for any crystal deformation. The numerical integration is done over a crystal domain where the electromagnetic waves propagate. The domain is divided into small regular cells whose vertices form the integration network. The kernel of our code is based on the programs developed by Gronkowski\textsuperscript{27} for applications in x-ray topography.

The amplitude of the diffracted and transmitted electric fields ($D_h$ and $D_0$, respectively) are given by the TT eqs.:

$$
\frac{\partial}{\partial \delta_0} D_0(\vec{r}) = -i \pi k \Psi_0 D_0(\vec{r}); \\
\frac{\partial}{\partial \delta_h} D_h(\vec{r}) = -i \pi k \Psi_0 D_0(\vec{r}) + 2 \pi i \left\{ k_\delta - \frac{\partial}{\partial \delta_h} (\vec{h} \cdot \vec{u}(\vec{r})) \right\} D_h(\vec{r}),
$$

(14)

where, $k$ is the wavevector in vacuum, $\vec{h}$ is the reciprocal lattice vector, $\beta_h = (|k_0|^2 - |k_h|^2)/(2|k|^2)$, $k_0$ and $k_h$ are diffracted and transmitted wavevectors, respectively; $\vec{u}$ is the displacement vector of the deformation.

The Eqs. (14) are expressed along a set of oblique axes $\hat{s}_0$ and $\hat{s}_h$ parallel to the transmitted and diffracted beam directions, respectively, inside the crystal (Fig. 3). The boundary conditions to be imposed at the $\Gamma_i$ surfaces of Fig. 3 are different in Laue and Bragg cases. Moreover, in the Bragg case different boundary conditions have to be set for thick and thin crystals.\textsuperscript{28} In order to ensure the continuity conditions at the entrance surface, and to include the absorption, the imaginary part of $k_0$ and $k_h$ are introduced. These vectors are conveniently chosen to be perpendicular to the crystal surface.\textsuperscript{29}

All the numerical solutions of the TT equations found until now are based on the finite difference method (FDM). The most used method is based on the half step derivative, proposed by Authier et al.\textsuperscript{30} The implementation of it
by Gronkowski is used in our code. It consists in writing the system in a recurrent matrix form:

\[
\begin{pmatrix}
D_0(s_0, s_h) \\
D_h(s_0, s_h)
\end{pmatrix} = E \begin{pmatrix}
C_2 & AC_2 & AB & AC_1 \\
B & AB & B & C_1
\end{pmatrix} \begin{pmatrix}
D_0(s_0 - p, s_h) \\
D_h(s_0 - p, s_h) \\
D_0(s_0 - p, s_h - q) \\
D_h(s_0 - p, s_h - q)
\end{pmatrix}
\]

(15)

where \( p \) and \( q \) are the elementary steps in \( s_0 \) and \( s_h \), respectively, and

\[
A = -\frac{1}{2} \pi i pk\Psi_R; \ B = -\frac{1}{2} \pi i qk\Psi_H; \ C_1 = 1+W; \ C_2 = 1-W; \ E = \frac{1}{1 - W - AB}; \ W = \beta_h - i\pi q \frac{\partial (\hat{n} \cdot \hat{u})}{\partial s_h} (s_0, s_h - \frac{q}{2})
\]

(16)

In Eq. (15) it is assumed that the amplitudes of the transmitted and diffracted waves in a given point \( R \) depend on the amplitudes at the points \( Q \) and \( P \) (Fig. 4). This is consistent with the hyperbolic nature of the TT equations, which means that the dependence domain of the point \( R \) is the triangle \( RQP \). The values of the wave amplitudes outside this triangle do not influence the wavefields in \( R \). The integration network and working principles are different for the Laue and Bragg cases. In order to simulate the incident wave, two limit cases are possible: the spherical wave and the plane wave. The first is simulated by one elementary point source in the integration network at the entrance surface \( \Gamma_1 \). The second is created by many coherent points in \( \Gamma_1 \). The accuracy of the results is very sensitive to
the sample of the incident wave. The phases of an incident wave with a large cross section oscillate very fast, thus, a constant-step integration network like the one we used needs many steps and consequently the processing time increases. This difficulty should be removed with the FEM. Some example of the results produced by our computer program are shown in Fig. 5.

![Figure 5](image.png)

**Figure 5.** Left: Comparison of diffraction profiles for Si 111 flat thick symmetrically cut crystal in Bragg geometry, $P = 1$, $E = 8\ kWV$, calculated with the TT code (solid) and the Zachariasen code (dashed). The last curves overlap perfectly. Center: diffraction profiles for Si 220 Laue flat symmetrical crystal, 50$\mu$m thick and $E = 8\ kWV$, calculated with the TT code (solid) and the Zachariasen code (dashed). Right: Diffraction profiles for a Si 111 crystal, $t = 0.525\ mm$, $\alpha = 55^\circ$, $\rho = 1.9\ m$, $E = 17.48\ kWV$ in Laue geometry. The PP calculation is overplotted with dashed line. The modelled data agree qualitatively with the experimental and calculated data from Suortti et al.$^{31}$

5. A NEW APPROACH TO SOLVE NUMERICALLY THE TAKAGI-TAUPIN EQUATIONS

In this paragraph we describe a novel approach to solve numerically the TT equations by using the Finite Element Method (FEM). An analogous computational scheme is described in Ref. 32, where it was successfully applied to solve a second order partial derivative equation by minimizing its known functional. Let us consider the region $\Omega$ (Borrman fan) shown in Fig. 3, with the boundaries $\Gamma_i$, $i = 1, \ldots, 4$, where $\Gamma_1$ is the entrance surface. The boundary conditions are fixed once the crystal geometry (Bragg or Laue case) has been set. If we define

$$\beta_{h'} = \beta_h - \frac{1}{k} \frac{\partial}{\partial s_h} (h \cdot \bar{u}(\bar{r}))$$

(17)

the eqs. (14) can be written in a compact form:

$$\frac{\partial}{\partial s_0} D_0(\bar{r}) = AD_h(\bar{r})$$

$$\frac{\partial}{\partial s_h} D_h(\bar{r}) = BD_0(\bar{r}) + C(\bar{r}) D_h(\bar{r})$$

(18)

where $A = -i \pi k \Psi_R, B = -i \pi k \Psi_H$ and $C(\bar{r}) = 2 \pi k \beta_{h'}(\bar{r})$.

By multiplying each side of Eq. (18) by a suitably chosen differentiable function $w$ ($w \in L^2$), and integrating over $\Omega$, one obtains:

$$\int_{\Omega} \frac{\partial D_0(\bar{r})}{\partial s_0} w d\Omega = \int_{\Omega} A D_h(\bar{r}) w d\Omega$$

$$\int_{\Omega} \frac{\partial D_h(\bar{r})}{\partial s_h} w d\Omega = \int_{\Omega} (B D_0(\bar{r}) + C(\bar{r}) D_h(\bar{r})) w d\Omega, \quad \forall w \in L^2.$$
Integrating the system (19) by parts and making use of the Green theorem, one obtains:

\[
\int_{\Omega} \frac{\partial w}{\partial \delta_0} D_0(\delta) d\Omega + \int_{\Omega} AD_h(\delta) w d\Omega - \int_{\Gamma_3} D_0(\delta) w d\Gamma = \int_{\Gamma_1} D_0(\delta) w d\Gamma
\]

\[
\int_{\Omega} \frac{\partial w}{\partial \delta_h} D_h(\delta) d\Omega + \int_{\Omega} (BD_0(\delta) + C(\delta) D_h(\delta)) w d\Omega - \int_{\Gamma_3} D_h(\delta) w d\Gamma = \int_{\Gamma_1} D_h(\delta) w d\Gamma. \tag{20}
\]

It can be shown that (20) and (18) are mathematically equivalent, namely a solution of (20) is also a solution of (18) and vice versa.

Let us introduce the coordinates \( x \) and \( z \) in (20), defined as:

\[
x = s_0 \sin \psi_0 = -s_h \sin \psi_h
\]

\[
z = s_0 \cos \psi_0 = s_h \cos \psi_h
\]

where \( \psi_0 \) and \( \psi_h \) are the angles which the directions \( \vec{s}_0 \) and \( \vec{s}_h \) form with the normal to the crystal surface, respectively (see Fig. 3). Taking into account that \( D_0 = D_h = 0 \) along \( \Gamma_2 \) and \( \Gamma_4 \) and that \( \vec{i}_z . d\Gamma \) (\( \vec{i}_z \) is the unit vector along the z direction) vanishes on \( \Gamma_1 \) and \( \Gamma_3 \), eq. (20) becomes:

\[
\int_{\Omega} D_0 \left[ \frac{\partial w}{\partial x} \sin \psi_0 + \frac{\partial w}{\partial z} \cos \psi_0 \right] d\Omega + \int_{\Omega} AD_h w d\Omega - \int_{\Gamma_3} D_0 \sin \psi_0 w d\Gamma = \int_{\Gamma_1} D_0 \sin \psi_0 w d\Gamma;
\]

\[
\int_{\Omega} D_h \left[ -\frac{\partial w}{\partial x} \sin \psi_h + \frac{\partial w}{\partial z} \cos \psi_h \right] d\Omega + \int_{\Omega} [BD_0 w + C(x, z) D_h w] d\Omega - \int_{\Gamma_3} D_h \sin \psi_h w d\Gamma = \int_{\Gamma_1} D_h \sin \psi_h w d\Gamma.
\] \tag{21}

We restrict now the possible choice of functions \( w \) to a limited set \( \{ N_i \} \), where the \( N_i \) (shape functions) are locally defined in the triangular elements of an automatically generated mesh over \( \Omega \).

The Eqs. (20) and (21) represent the weak form of the TT equations and serve as a starting point for the well known Rayleigh-Ritz procedure by mean of which an approximate solution under given boundary conditions is found. In particular, solutions \( D_0 \) and \( D_h \) are sought of the type:

\[
D_0 = \sum_{i=1}^{N} N_i(\delta) S_i; \quad D_h = \sum_{i=1}^{N} N_i(\delta) T_i \tag{22}
\]

The upper limit \( N \) of the sums in (22) is the number of knots associated to an element, \( S_i \) and \( T_i \) are the \( 2N \) weighting coefficients which are to be determined numerically. We shall call \( K_j \) the set of triangles to which the \( j \)-th knot belongs and indicate with \( l \) the generic triangle of area \( \Delta_l \) belonging to the set \( K_j \). Furthermore we put:

\[
g_i = \int_{\Delta_l} N_i d\Omega; \quad p_i = \int_{\Delta_l} N_i d\Omega; \quad r_i = \int_{\Delta_l} C(x, y) N_i d\Omega; \quad (i = 1, 2, 3) \tag{23}
\]

where \( N_i \) denotes the function \( N_j \) in the \( i \)-th knot of the \( l \)-th triangle.

It has to be noticed that, being \( N_j \neq 0 \) only if the \( j \)-th node belongs to \( \Gamma_i \), the line integrals in (21) are restricted to the two boundary points (say \( \alpha \) and \( \beta \)) of the mesh related to the \( j \)-th node. By approximating the line integrals on the left hand-side of Eqs. (21) by means of the trapezoidal rule, we obtain:

\[
\int_{\alpha}^{\beta} \left( \sum_{j} N_j S_j \right) N_j \sin \psi_0 d\Gamma = \left( \frac{x_j - x_{\alpha}}{6} S_a + \frac{x_j - x_{\beta}}{6} S_{\beta} + \frac{x_{\beta} - x_{\alpha}}{3} S_j \right) \sin \psi_0, \tag{24}
\]

and:

\[
\int_{\alpha}^{\beta} \left( \sum_{j} N_j S_j \right) N_j \sin \psi_h d\Gamma = \left( \frac{x_j - x_{\alpha}}{6} T_a + \frac{x_j - x_{\beta}}{6} T_{\beta} + \frac{x_{\beta} - x_{\alpha}}{3} T_j \right) \sin \psi_h. \tag{25}
\]
One obtains analogous results for the line integrals on the right hand side of Eq. (21). For sake of compactness we express the system (21) in matrix form:

\[
\begin{pmatrix}
A_1 \\
A_2
\end{pmatrix}
\begin{pmatrix}
S \\
T
\end{pmatrix} =
\begin{pmatrix}
B_1 \\
B_2
\end{pmatrix}
\]

(26)

These will be shown later in this section. Taking into account Eq. (24) and Eq. (25) the j-th rows \(A_{1j}\) and \(A_{2j}\) of the sub-matrices \(A_1\) and \(A_2\), respectively, can be written as:

\[
A_{1j} = \sum_{i \in K_j} \left[ \left( \frac{\partial N_j}{\partial x} \sin \psi_0 + \frac{\partial N_j}{\partial z} \cos \psi_0 \right) \sum_{i=1}^3 p_i S_i + A \sum_{i=1}^3 q_i T_i \right] + 
\left( \frac{x_j - x_a}{6} S_a + \frac{x_j - x_b}{3} S_b \right) \sin \psi_0
\]

(27)

\[
A_{2j} = \sum_{i \in K_j} \left[ \left( -\frac{\partial N_j}{\partial x} \sin \psi_h + \frac{\partial N_j}{\partial z} \cos \psi_h \right) \sum_{i=1}^3 p_i T_i + B \sum_{i=1}^3 q_i S_i + \sum_{i=1}^3 r_i T_i \right] + 
\left( \frac{x_j - x_a}{6} T_a + \frac{x_j - x_b}{3} T_b \right) \sin \psi_h
\]

(28)

We consider the case where the coefficients \(S_i\) and \(T_i\) (also called knot variables) are assigned the values of the functions in the knot points. As the expressions (22) must hold for any arbitrary choice of the knot variables, the functions \(N_i(r_j)\) must meet the condition:

\[
N_i(r_j) = \begin{cases} 
1 & j = 1 \\
0 & j \neq i 
\end{cases}
\]

(29)

on every knot of the discretized domain. For every triangle, a local coordinate system \(L_i(i = 1, 2, 3)\) can be introduced such that:

\[
0 \leq L_k \leq 1 \quad (k = 1, 2, 3); \\
L_1 + L_2 + L_3 = 1.
\]

(30)

If three knot points \(P_k(x_k, z_k)\) are set on every triangle vertex, one can express their coordinates in the local system (30) as:

\[
x = L_1 x_1 + L_2 x_2 + L_3 x_3; \quad z = L_1 z_1 + L_2 z_2 + L_3 z_3.
\]

(31)

Solving for \(L_1, L_2, L_3\) one obtains:

\[
L_k = (a_k + b_k x + c_k z)/(2\Delta) \quad (k = 1, 2, 3),
\]

(32)

where:

\[
a_1 = x_2 z_3 - x_3 z_2; \quad b_1 = z_2 - z_3; \quad c_1 = x_3 - x_2; \\
a_2 = x_3 z_1 - x_1 z_3; \quad b_2 = z_3 - z_1; \quad c_2 = x_1 - x_3; \\
a_3 = x_1 z_2 - x_2 z_1; \quad b_3 = z_1 - z_2; \quad c_3 = x_2 - x_1,
\]

and \(\Delta = (a_1 + a_2 + a_3)/2\) is the triangle area. Equating the \(N_i\) functions to the \(L_i\)'s defined in (32) we obtain the following expressions for \(p_i, q_i,\) and \(r_i:\)

\[
p_i = \frac{p_i}{\Delta} = \int_{\Delta_i} L_i \, d\Omega_i = \frac{A_i}{2}
\]

(33)

\[
q_i = \frac{q_i}{\Delta} = \int_{\Delta_i} L_i \, L_j \, d\Omega_i = \frac{A_{ij}}{12}
\]

(34)

\[
r_i = r_i = \int_{\Delta_i} C \left( x_i^2 + y_i^2 + z_i^2 \right) L_i \, L_j \, d\Omega_i = C(pM) \frac{A_i}{12}
\]

(35)
In (35) the function $C(x, z)$ has been approximated by its value in the triangle middle joint $p_M$. Under the above assumptions, (27) and (28) can be rewritten as:

$$A_{1j} = \sum_{l \in K_j} \frac{b_l \sin \psi_0 + c_l \cos \psi_0}{2 \Delta_l} \frac{\Delta_l^3}{3} \sum_{i=1}^{3} S_i + A \frac{\Delta_l}{12} \sum_{i=1}^{3} T_i +$$

$$- \left( \frac{x_j - x_\alpha}{6} S_\alpha + \frac{x_\beta - x_j}{6} S_\beta + \frac{x_j - x_\alpha}{3} S_j \right) \sin \psi_0,$$

$$A_{2j} = \sum_{l \in K_j} \frac{-b_l \sin \psi_h + c_l \cos \psi_h}{2 \Delta_l} \frac{\Delta_l^3}{3} \sum_{i=1}^{3} T_i + B \frac{\Delta_l}{12} \sum_{i=1}^{3} S_i + C(p_M) \frac{\Delta_l}{12} \sum_{i=1}^{3} T_i +$$

$$\left( \frac{x_j - x_\alpha}{6} T_\alpha + \frac{x_\beta - x_j}{6} T_\beta + \frac{x_j - x_\alpha}{3} T_j \right) \sin \psi_h, \quad K_j = 1, \ldots, N,$$

where the last terms of the expression (36) are equal to zero if $j \notin \Gamma_3$. The $j$-th rows $B_{1j}$ and $B_{2j}$ of the vectors $B_1$ and $B_2$ in (26) write:

$$\begin{cases}
B_{1j} = 0, & j \notin \Gamma_1 \\
B_{1j} = \left( \frac{x_\alpha - x_j}{6} S_\alpha + \frac{x_j - x_\alpha}{6} S_\beta + \frac{x_\alpha - x_j}{3} S_j \right) \sin \psi_0, & j \in \Gamma_1
\end{cases}$$

and:

$$\begin{cases}
B_{2j} = 0, & j \notin \Gamma_1 \\
B_{2j} = - \left( \frac{x_\alpha - x_j}{6} T_\alpha + \frac{x_j - x_\alpha}{6} T_\beta + \frac{x_\alpha - x_j}{3} T_j \right) \sin \psi_h, & j \in \Gamma_1
\end{cases}$$

As one may easily notice, owing to the particular choice of the shape functions $L_k$ the weak form of the TT equations reduces to a linear algebraic system of $2N$ (generally a large number) equations which has to be solved for the unknown variables $S_i$ and $T_i$. The system matrix $\begin{pmatrix} A_1 & A_2 \end{pmatrix}$ is sparse because its elements are non-zero only if the $i$-th and $j$-th nodes are connected to each other. The system (26) has been coded in a prototype software package written in MATLAB.

We have already mentioned some advantageous features of the FEM. It should also be added here the ability of generating an adaptive mesh automatically by minimizing a given error function. Moreover, the boundary conditions are, as it follows from the previous description, naturally included in the solving algorithm. The FEM code is currently under development at the ESRF. It has been tested to map the values of the electrical field inside and at
the surface of a flat perfect crystal (see Fig. 6). It was also used to simulate the topograph of a flat crystal with a spherical inclusion.

In the next future we will focus our development on simulations of diffraction properties of bent crystals without and with defects in order to reproduce the experimental reflectivity curves of thin and thick crystals in Laue and Bragg geometry.

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