PyTTE: The Technical Document
Version 0.2

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1 Introduction

PyTTE (pronounced *pie-tee-tee-ee*) is a Python package for solving X-ray diffraction curves of bent crystals in reflection and transmission geometries. The computation of the diffraction curves is based on the numerical integration of 1D Takagi-Taupin equation (TTE) which is derived from a more general Takagi-Taupin theory describing the propagation of electromagnetic waves in a (quasi)periodic medium. Both energy and angle scans are supported. This document describes the theoretical basis behind PyTTE.

2 Takagi-Taupin equation

In the typical two-beam case, the Takagi-Taupin equations are can be written as

$$\begin{cases} \dfrac{\partial D_0}{\partial s_0} = ic_0 D_0 + ic_{\bar{h}} D_h & \text{(1a)} \\ \dfrac{\partial D_h}{\partial s_h} = i\left(c_0 + \beta + \dfrac{\partial(\mathbf{h}\cdot\mathbf{u})}{\partial s_h}\right) D_h + ic_h D_0, & \text{(1b)} \end{cases}$$

where D_0 and D_h are the pseudoamplitudes of the incident and diffracted waves, and s_0 and s_h coordinates along their direction of propagation, respectively. The deformation of the crystal is contained in $\mathbf{h}\cdot\mathbf{u}$ which will be considered in detail later. The coefficients $c_{0,h,\bar{h}}$ are given by

$$c_0 = \frac{k\chi_0}{2} \qquad c_{h,\bar{h}} = \frac{kC\chi_{h,\bar{h}}}{2}, \tag{2}$$

where $k = 2\pi/\lambda$ and $C = 1$ for σ-polarization and $\cos 2\theta_B$ for π-polarization. The deviation parameter $\beta = (k_h^2 - k_0^2)/2k_h$ is quite often approximated by $\beta \approx k\Delta\theta \sin 2\theta_B$, where $\Delta\theta$ is the deviation from the Bragg angle. However, since this approximation ceases to be valid near the backscattering condition, PyTTE uses a more general form

$$\beta = \frac{2\pi}{d_h}\left(\frac{\lambda}{2d_h} - \sin\theta\right) = h\left(\frac{\lambda}{2d_h} - \sin\theta\right), \tag{3}$$

where d_h is the interplanar separation of the diffractive planes corresponding to the reciprocal vector $\mathbf{h}$ and θ is the incidence angle relative to the aforementioned planes.

The partial derivatives with respect to s_0 and s_h can be written in Cartesian coordinates as

$$\frac{\partial}{\partial s_0} = \cos\alpha_0 \frac{\partial}{\partial x} - \sin\alpha_0 \frac{\partial}{\partial z} \qquad \frac{\partial}{\partial s_h} = \cos\alpha_h \frac{\partial}{\partial x} + \sin\alpha_h \frac{\partial}{\partial z}. \tag{4}$$

The incidence and exit angles α_0 and α_h with respect to the crystal surface are related to θ by $\alpha_0 = \theta + \varphi$ and $\alpha_h = \theta - \varphi$, where φ is the asymmetry angle (positive clockwise). When seeking a solely depth-dependent solution for D_0 and D_h, we may drop the x-derivatives and thus obtain

$$\begin{cases} \dfrac{dD_0}{dz} = -i\gamma_0 c_0 D_0 - i\gamma_0 c_{\bar{h}} D_h & \text{(5a)} \\ \dfrac{dD_h}{dz} = i\gamma_h \left(c_0 + \beta + \dfrac{\partial(\mathbf{h}\cdot\mathbf{u})}{\partial s_h} \right) D_h + i\gamma_h c_h D_0, & \text{(5b)} \end{cases}$$

where $\gamma_0 = 1/\sin\alpha_0$ and $\gamma_h = 1/\sin\alpha_h$. By defining $\xi = D_h/D_0$, the equations can be written as a single ordinary differential equation

$$\frac{d\xi}{dz} = i\gamma_0 c_{\bar{h}} \xi^2 + i\left[(\gamma_0 + \gamma_h) c_0 + \gamma_h \beta + \gamma_h \frac{\partial(\mathbf{h}\cdot\mathbf{u})}{\partial s_h} \right] \xi + i\gamma_h c_h \tag{6}$$

In the reflection geometry (*i.e.* the Bragg case), the reflectivity R of the crystal with thickness t can be solved by integrating Equation (6) from the bottom of the crystal $z = -t$ to the top surface $z = 0$. The initial condition is set $\xi(-t) = 0$. The reflectivity, which is defined in the terms of integrated intensity, is then computed $R = \gamma_0/\gamma_h |\xi(0)|^2$ where γ_0/γ_h takes care of different footprint sizes in the asymmetric case. Using the solved ξ and Equation (5a), the transmission $T = |D_0(-t)/D_0(0)|^2$ can be then solved from

$$\frac{dD_0}{dz} = -i\left(\gamma_0 c_0 + \gamma_0 c_{\bar{h}} \xi\right) D_0 \tag{7}$$

by integrating from $z = 0$ to $z = -t$. The transmission geometry (the Laue case) is more straightforward, as the ODEs for ξ and D_0 can be integrated simultaneously from $z = 0$ to $z = -t$. With the initial conditions are set $\xi(0) = 0$ and $D_0(0) = 1$, the forward-diffracted intensity at the exit surface is $|D_0(-t)|^2$ and the diffracted intensity is $|D_h(-t)|^2 = |\xi(-t) D_0(-t)|^2$.

3 Deformation

As stated in the previous section, the deformation is introduced through $\partial_h(\mathbf{h}\cdot\mathbf{u})$ term where $\mathbf{u}$ is the displacement vector field. Taking the asymmetry into account, the reciprocal vector is given by $\mathbf{h} = h\sin\varphi\hat{\mathbf{x}} + h\cos\varphi\hat{\mathbf{z}}$. Thus

$$\frac{\partial(\mathbf{h}\cdot\mathbf{u})}{\partial s_h} = h\sin\varphi\frac{\partial u_x}{\partial s_h} + h\cos\varphi\frac{\partial u_z}{\partial s_h}. \tag{8}$$

Again we write the partial derivatives in terms of x and z. In this case, however, neither x- or z-derivatives can be dropped as they both contain physical information about the rotation and the separation of the diffractive planes. Since the beam propagates also in the x-direction, the situation is not strictly speaking one dimensional. However, since the x-coordinate is geometrically related to z, the problem can be treated as such. Therefore the deformation term becomes

$$\frac{\partial(\mathbf{h}\cdot\mathbf{u})}{\partial s_h} = h\left(\sin\varphi\cos\alpha'\frac{\partial u_x}{\partial x} + \sin\varphi\sin\alpha'\frac{\partial u_x}{\partial z} + \cos\varphi\cos\alpha'\frac{\partial u_z}{\partial x} + \cos\varphi\sin\alpha'\frac{\partial u_z}{\partial z} \right), \tag{9}$$

where the derivatives, that are functions of x and z, are made only z-dependent with $x(z) = -z\cot\alpha$. PyTTE computes the strain term from the Jacobian of $\mathbf{u}$.

3.1 Anisotropic plate

According to [1], the components of the displacement field for an anisotropic plate bent by two (scaled) torques m_x and m_y are

$$u_x = (S_{11}m_x + S_{12}m_y)xz + (S_{51}m_x + S_{52}m_y)\frac{z^2}{2} + (S_{61}m_x + S_{62}m_y)\frac{yz}{2} \tag{10}$$

$$u_y = (S_{21}m_x + S_{22}m_y)yz + (S_{41}m_x + S_{42}m_y)\frac{z^2}{2} + (S_{61}m_x + S_{62}m_y)\frac{xz}{2} \tag{11}$$

$$u_z = -(S_{11}m_x + S_{12}m_y)\frac{x^2}{2} - (S_{21}m_x + S_{22}m_y)\frac{y^2}{2} - (S_{61}m_x + S_{62}m_y)\frac{xy}{2} + (S_{31}m_x + S_{32}m_y)\frac{z^2}{2}, \tag{12}$$

where S_{ij} are the components of the compliance matrix. Thus we find the partial derivatives:

$$\frac{\partial u_x}{\partial x} = (S_{11}m_x + S_{12}m_y)z \tag{13}$$

$$\frac{\partial u_x}{\partial z} = (S_{11}m_x + S_{12}m_y)x + (S_{51}m_x + S_{52}m_y)z + (S_{61}m_x + S_{62}m_y)\frac{y}{2} \tag{14}$$

$$\frac{\partial u_z}{\partial x} = -(S_{11}m_x + S_{12}m_y)x - (S_{61}m_x + S_{62}m_y)\frac{y}{2} \tag{15}$$

$$\frac{\partial u_z}{\partial z} = (S_{31}m_x + S_{32}m_y)z \tag{16}$$

The torques are related to the bending radii R_i by[1]

$$\frac{1}{R_x} = -S_{11}m_x - S_{12}m_y, \qquad \frac{1}{R_y} = -S_{21}m_x - S_{22}m_y. \tag{17}$$

Thus

$$m_x = \frac{1}{S_{11}S_{22} - S_{12}S_{21}}\left(\frac{S_{12}}{R_y} - \frac{S_{22}}{R_x}\right), \qquad m_y = \frac{1}{S_{11}S_{22} - S_{12}S_{21}}\left(\frac{S_{21}}{R_x} - \frac{S_{11}}{R_y}\right). \tag{18}$$

3.2 Isotropic plate

The general anisotropic equations simplify considerably when assuming the plate to be isotropic. The isotropic compliance matrix is given by

$$S = \frac{1}{E}\begin{bmatrix} 1 & -\nu & -\nu & 0 & 0 & 0 \\ -\nu & 1 & -\nu & 0 & 0 & 0 \\ -\nu & -\nu & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(1+\nu) & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(1+\nu) & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(1+\nu) \end{bmatrix}, \tag{19}$$

where E is Young's modulus and ν is the Poisson ratio. Plugging these into (18), we obtain

$$m_x = -\frac{E}{1-\nu^2}\left(\frac{1}{R_x} + \frac{\nu}{R_y}\right), \qquad m_y = -\frac{E}{1-\nu^2}\left(\frac{1}{R_y} + \frac{\nu}{R_x}\right) \tag{20}$$

and thus

$$\frac{\partial u_x}{\partial x} = -\frac{z}{R_x}, \qquad \frac{\partial u_x}{\partial z} = -\frac{x}{R_x}, \qquad \frac{\partial u_z}{\partial x} = \frac{x}{R_x}, \qquad \frac{\partial u_z}{\partial z} = \frac{\nu}{1-\nu}\left(\frac{1}{R_x} + \frac{1}{R_y}\right)z. \tag{21}$$

Finally, since PyTTE assumes the top surface is at $z = 0$, we need to shift the z-axis $z \to z + t/2$

[1] In this work the signs of R_i is the opposite to that of [1]

4 Crystallography and elastic constants

4.1 Crystallographic vectors

For crystallographic data, PYTTE v. 0.2 relies on the internal library of XRAYLIB[2]. The direct primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ given in a Cartesian system are calculated from the lattice parameters a,b,c, α, β, and γ as follows

$$\mathbf{a}_1 = a\begin{bmatrix}1\\0\\0\end{bmatrix} \qquad \mathbf{a}_2 = b\begin{bmatrix}\cos\gamma\\\sin\gamma\\0\end{bmatrix} \qquad \mathbf{a}_3 = \frac{c}{\sin\gamma}\begin{bmatrix}\cos\beta\sin\gamma\\\cos\alpha-\cos\beta\cos\gamma\\\sqrt{\sin^2\gamma-\cos^2\alpha-\cos^2\beta+2\cos\alpha\cos\beta\cos\gamma}\end{bmatrix} \tag{22}$$

The reciprocal primitive vectors are calculated according to

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2\times\mathbf{a}_3}{|\mathbf{a}_1\times\mathbf{a}_2\cdot\mathbf{a}_3|} \qquad \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3\times\mathbf{a}_1}{|\mathbf{a}_1\times\mathbf{a}_2\cdot\mathbf{a}_3|} \qquad \mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1\times\mathbf{a}_2}{|\mathbf{a}_1\times\mathbf{a}_2\cdot\mathbf{a}_3|}. \tag{23}$$

The reciprocal vector $\mathbf{h}$ corresponding and normal to the Bragg planes with the Miller indices (h,k,l) is thus

$$\mathbf{h} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3. \tag{24}$$

Crystal directions $[n_1n_2n_3]$ are converted to Cartesian vectors (x,y,z) followingly

$$\begin{bmatrix}x\\y\\z\end{bmatrix} = \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 & \mathbf{a}_3\end{bmatrix}\begin{bmatrix}n_1\\n_2\\n_3\end{bmatrix} \tag{25}$$

and *vice versa* by inverting $[\mathbf{a}_1\ \mathbf{a}_2\ \mathbf{a}_3]$.

4.2 Vector and tensor rotation

A general counterclockwise rotation by θ about axis $\mathbf{u} = (u_1,u_2,u_3)$, with $|\mathbf{u}| = 1$, is given by the matrix

$$Q(\mathbf{u},\theta) = \begin{bmatrix}\cos\theta+u_1^2(1-\cos\theta) & u_1u_2(1-\cos\theta)-u_3\sin\theta & u_1u_3(1-\cos\theta)+u_2\sin\theta\\ u_2u_1(1-\cos\theta)+u_3\sin\theta & \cos\theta+u_2^2(1-\cos\theta) & u_2u_3(1-\cos\theta)-u_1\sin\theta\\ u_3u_1(1-\cos\theta)-u_2\sin\theta & u_3u_2(1-\cos\theta)+u_1\sin\theta & \cos\theta+u_3^2(1-\cos\theta)\end{bmatrix}, \tag{26}$$

also known as Rodrigues' rotation formula. Rotation is applied to vector $\mathbf{v}$ by the ordinary matrix multiplication $Q\mathbf{v}$. For a 4th order tensor t, the rotated components are

$$t'_{ijkl} = \sum_{p,q,r,s} Q_{ip}Q_{jq}Q_{kr}Q_{ls}t_{pqrs}. \tag{27}$$

In PYTTE, it is taken that $\mathbf{h} \parallel \hat{\mathbf{z}}$, *i.e.* the symmetric Bragg case, corresponds to the asymmetry angle $\phi = 0$. Thus in the most general case the elastic tensors go through the following three rotations:

1. Rotate elastic tensors and direction vectors so that $\mathbf{h}$ is parallel to z-axis
2. Apply a rotation about z-axis to align the crystal directions in xy-plane
3. Apply the asymmetry by performing the rotation of ϕ about y-axis.

Assuming that at least either of h an k is non-zero, the rotation of $\mathbf{h} = (h_1, h_2, h_3)$ (step 1) is performed with the following axis and angle

$$\mathbf{u} = \frac{1}{\sqrt{h_1^2 + h_2^2}} \begin{bmatrix} h_2 \\ -h_1 \\ 0 \end{bmatrix} \qquad \theta = \arccos\left(\frac{h_3}{\sqrt{h_1^2 + h_2^2 + h_3^2}}\right). \tag{28}$$

If $h = k = 0$, a rotation of $\theta = \pi$ about $\mathbf{u} = -\hat{\mathbf{y}}$ is applied when $l < 0$; no rotation is needed for $l > 0$. For the in-plane rotation (step 2), the axis is $\mathbf{u} = [0, 0, 1]^{\mathrm{T}}$ and for the asymmetry rotation (step 3) $\mathbf{u} = [0, 1, 0]^{\mathrm{T}}$ and $\theta = \phi$.[2]

References

[1] Manuel Sanchez del Rio, Nicolas Perez-Bocanegra, Xianbo Shi, Veijo Honkimäki, and Lin Zhang. Simulation of x-ray diffraction profiles for bent anisotropic crystals. *Journal of Applied Crystallography*, 48(2):477–491, mar 2015.

[2] Tom Schoonjans, Antonio Brunetti, Bruno Golosio, Manuel Sanchez del Rio, Vicente Armando Solé, Claudio Ferrero, and Laszlo Vincze. The xraylib library for x-ray–matter interactions. recent developments. *Spectrochimica Acta Part B: Atomic Spectroscopy*, 66:776–784, 2011. doi:10.1016/j.sab.2011.09.011.

[2] Note that ϕ is defined clockwise-positive but about $-\hat{\mathbf{y}}$, not $\hat{\mathbf{y}}$