PyTTE: The Technical Document

Ari-Pekka Honkanen

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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 $\mathbf{u}$.