TBCALC: The Technical Document
Version 1.0

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1 Introduction

This documentation describes briefly the technical details and theoretical basis of TBCALC package used to calculate the X-ray diffraction curves of toroidally bent, Johann-type crystal analysers. For comprehensive explanation, please refer to [1].

2 Calculation of the reflectivity curves

As formally shown [2], the effect of a constant component in a strain field to the diffraction curve can be taken into account by a applying a shift, either in energy or angle domain, to the Takagi-Taupin curve calculated without it. Since for toroidally bent crystal analysers the total strain field can be divided into a sum of depth-dependent and transversally varying parts, this allows efficient calculation of the reflectivity curves even for very large wafers. The calculation is summed up in the following steps:

- Compute the 1D Takagi-Taupin curve for the depth-dependent component of the strain field. TBCALC uses another Python package PYTTE for this.
- Calculate distribution the energy or angle shifts due to the transversally varying component. The Johann error can be included in this part.
- Convolve the 1D TT-curve with the shift distribution to obtain the full reflectivity curve of the analyser.
- Convolve the result with the incident bandwidth, if needed.

2.1 Depth-dependent Takagi-Taupin curve

The 1D TT-curve is calculated using PyTTE. In v. 1.0 of TBCALC it is assumed that the main axes of curvature of TBCA:s are along the meridional and sagittal directions with respect to the diffraction plane and coincide, respectively, with the x- and y-axes of the Cartesian system used in the code and the manuscript [1]. By default, the internal anisotropic compliance matrices[1] are used for elastic parameters and XRAYLIB[2] for crystallograpic parameters and structure factors.

[1] Values from CRC Handbook of Chemistry and Physics, 82nd edition (2001)

[2] `https://github.com/tschoonj/xraylib`

2.2 Transverse stress and strain tensor fields

For convenience, this section lists the equations for the transverse stress tensor and the strain it causes. Refer to [1] for the derivation and discussion.

2.2.1 Isotropic circular

The components of the transverse stress tensor of an isotropic circular wafer with the diameter L and meridional and sagittal bending radii R_1 and R_2, respectively, are

$$\sigma_{xx} = \frac{E}{16R_1R_2}\left(\frac{L^2}{4} - x^2 - 3y^2\right) \qquad \sigma_{xy} = \frac{E}{8R_1R_2}xy \qquad \sigma_{yy} = \frac{E}{16R_1R_2}\left(\frac{L^2}{4} - 3x^2 - y^2\right) \tag{1}$$

the corresponding strain tensor components

$$u_{xx} = \frac{1}{16R_1R_2}\left[(1-\nu)\frac{L^2}{4} - (1-3\nu)x^2 - (3-\nu)y^2\right] \tag{2}$$

$$u_{yy} = \frac{1}{16R_1R_2}\left[(1-\nu)\frac{L^2}{4} - (1-3\nu)y^2 - (3-\nu)x^2\right] \tag{3}$$

$$u_{xy} = \frac{1+\nu}{8R_1R_2}xy \qquad u_{xz} = u_{yz} = 0 \qquad u_{zz} = \frac{\nu}{4R_1R_2}\left(x^2 + y^2 - \frac{L^2}{8}\right) \tag{4}$$

and the contact force per unit area

$$P = \frac{Ed}{16R_1^2R_2^2}\left[(3R_1 + R_2)\,x^2 + (R_1 + 3R_2)\,y^2 - (R_1 + R_2)\,\frac{L^2}{4}\right]. \tag{5}$$

2.2.2 Anisotropic circular

The stretching stress tensor components are

$$\sigma_{xx} = \frac{E'}{16R_1R_2}\left(\frac{L^2}{4} - x^2 - 3y^2\right) \quad \sigma_{yy} = \frac{E'}{16R_1R_2}\left(\frac{L^2}{4} - 3x^2 - y^2\right) \quad \sigma_{xy} = \frac{E'}{8R_1R_2}xy \tag{6}$$

where

$$E' = \frac{8}{3(S_{11} + S_{22}) + 2S_{12} + S_{66}}, \tag{7}$$

the corresponding strain tensor

$$u_{xx} = \frac{E'}{16R_1R_2}\left[(S_{11} + S_{12})\frac{L^2}{4} - (S_{11} + 3S_{12})x^2 - (3S_{11} + S_{12})y^2 + 2S_{16}xy\right] \tag{8}$$

$$u_{yy} = \frac{E'}{16R_1R_2}\left[(S_{21} + S_{22})\frac{L^2}{4} - (S_{21} + 3S_{22})x^2 - (3S_{21} + S_{22})y^2 + 2S_{26}xy\right] \tag{9}$$

$$u_{zz} = \frac{E'}{16R_1R_2}\left[(S_{31} + S_{32})\frac{L^2}{4} - (S_{31} + 3S_{32})x^2 - (3S_{31} + S_{32})y^2 + 2S_{36}xy\right] \tag{10}$$

$$u_{xz} = \frac{E'}{32R_1R_2}\left[(S_{41} + S_{42})\frac{L^2}{4} - (S_{41} + 3S_{42})x^2 - (3S_{41} + S_{42})y^2 + 2S_{46}xy\right] \tag{11}$$

$$u_{yz} = \frac{E'}{32R_1R_2}\left[(S_{51} + S_{52})\frac{L^2}{4} - (S_{51} + 3S_{52})x^2 - (3S_{51} + S_{52})y^2 + 2S_{56}xy\right] \tag{12}$$

$$u_{xy} = \frac{E'}{32R_1R_2}\left[(S_{61} + S_{62})\frac{L^2}{4} - (S_{61} + 3S_{62})x^2 - (3S_{61} + S_{62})y^2 + 2S_{66}xy\right] \tag{13}$$

and the contact force per unit area

$$P = \frac{E'd}{16R_1^2R_2^2}\left[(3R_1+R_2)\,x^2+(R_1+3R_2)\,y^2-(R_1+R_2)\,\frac{L^2}{4}\right]. \tag{14}$$

2.2.3 Isotropic rectangular

The components of the transverse stress tensor of an isotropic rectangular wafer with the side lengths a and b aligned with the meridional and sagittal radii of curvature R_1 and R_2, respectively, are

$$\sigma_{xx} = \frac{E}{gR_1R_2}\left[\frac{a^2}{12}-x^2+\left(\frac{1+\nu}{2}+5\frac{a^2}{b^2}+\frac{1-\nu}{2}\frac{a^4}{b^4}\right)\left(\frac{b^2}{12}-y^2\right)\right] \tag{15}$$

$$\sigma_{yy} = \frac{E}{gR_1R_2}\left[\frac{b^2}{12}-y^2+\left(\frac{1+\nu}{2}+5\frac{b^2}{a^2}+\frac{1-\nu}{2}\frac{b^4}{a^4}\right)\left(\frac{a^2}{12}-x^2\right)\right] \tag{16}$$

$$\sigma_{xy} = \frac{2E}{gR_1R_2}xy, \tag{17}$$

where

$$g = 8+10\left(\frac{a^2}{b^2}+\frac{b^2}{a^2}\right)+(1-\nu)\left(\frac{a^2}{b^2}-\frac{b^2}{a^2}\right)^2. \tag{18}$$

The stretching strain tensor components are

$$u_{xx}=\frac{\sigma_{xx}-\nu\sigma_{yy}}{E}\quad u_{yy}=\frac{\sigma_{yy}-\nu\sigma_{xx}}{E}\quad u_{xy}=\frac{1+\nu}{E}\sigma_{xy}\quad u_{xz}=u_{yz}=0\quad u_{zz}=-\frac{\nu}{E}(\sigma_{xx}+\sigma_{yy}) \tag{19}$$

and the contact force

$$P = -\frac{Ed}{gR_1^2R_2^2}\left[\left(R_1\left(\frac{1+\nu}{2}+5\frac{b^2}{a^2}+\frac{1-\nu}{2}\frac{b^4}{a^4}\right)+R_2\right)\left(\frac{a^2}{12}-x^2\right)\right.$$
$$\left.+\left(R_2\left(\frac{1+\nu}{2}+5\frac{a^2}{b^2}+\frac{1-\nu}{2}\frac{a^4}{b^4}\right)+R_1\right)\left(\frac{b^2}{12}-y^2\right)\right] \tag{20}$$

2.2.4 Anisotropic rectangular

For an anisotropic rectangular wafer, the transverse stress tensor components are

$$\sigma_{xx} = C_{02}+12C_{22}x^2+24C_{13}xy+12C_{04}y^2 \tag{21}$$

$$\sigma_{yy} = C_{20}+12C_{22}y^2+24C_{31}xy+12C_{40}x^2 \tag{22}$$

$$\sigma_{xy} = -C_{11}-12C_{31}x^2-24C_{22}xy-12C_{13}y^2 \tag{23}$$

from which we can calculate the corresponding strain tensor

$$u_{xx} = S_{11}\sigma_{xx}+S_{12}\sigma_{yy}+S_{16}\sigma_{xy} \tag{24}$$

$$u_{yy} = S_{21}\sigma_{xx}+S_{22}\sigma_{yy}+S_{26}\sigma_{xy} \tag{25}$$

$$u_{xy} = \frac{1}{2}\left(S_{61}\sigma_{xx}+S_{62}\sigma_{yy}+S_{66}\sigma_{xy}\right) \tag{26}$$

$$u_{xz} = \frac{1}{2}\left(S_{41}\sigma_{xx}+S_{42}\sigma_{yy}+S_{46}\sigma_{xy}\right) \tag{27}$$

$$u_{yz} = \frac{1}{2}\left(S_{51}\sigma_{xx}+S_{52}\sigma_{yy}+S_{56}\sigma_{xy}\right) \tag{28}$$

$$u_{zz} = S_{31}\sigma_{xx}+S_{32}\sigma_{yy}+S_{36}\sigma_{xy} \tag{29}$$

and the contact force per surface area

$$P = -d\left(\frac{\sigma_{xx}}{R_1} + \frac{\sigma_{yy}}{R_2}\right). \tag{30}$$

The coefficients C_{ij} are obtained by solving the matrix equation $\Lambda\mathbf{C} = \mathbf{b}$ in terms of $\mathbf{C}$ where

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{20} & C_{02} & C_{22} & C_{31} & C_{13} & C_{40} & C_{04} & \lambda_1 \end{bmatrix}^{\mathrm{T}}, \tag{31}$$

$$\mathbf{b} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -(24R_1R_2)^{-1} \end{bmatrix}^{\mathrm{T}}, \tag{32}$$

and

$$\Lambda = \begin{bmatrix} S_{66} & -S_{26} & -S_{16} & \Lambda_{14} & S_{66}a^2 & S_{66}b^2 & -S_{26}a^2 & -S_{16}b^2 & 0 \\ -S_{26} & S_{22} & S_{12} & \Lambda_{24} & -S_{26}a^2 & -S_{26}b^2 & S_{22}a^2 & S_{12}b^2 & 0 \\ -S_{16} & S_{12} & S_{11} & \Lambda_{34} & -S_{16}a^2 & -S_{16}b^2 & S_{12}a^2 & S_{11}b^2 & 0 \\ \Lambda_{41} & \Lambda_{42} & \Lambda_{43} & \Lambda_{44} & \Lambda_{45} & \Lambda_{46} & \Lambda_{47} & \Lambda_{48} & \Lambda_{49} \\ 5S_{66}a^2 & -5S_{26}a^2 & -5S_{16}a^2 & \Lambda_{54} & \Lambda_{55} & \Lambda_{56} & -9S_{26}a^4 & -5S_{16}a^2b^2 & -2S_{26} \\ 5S_{66}b^2 & -5S_{26}b^2 & -5S_{16}b^2 & \Lambda_{64} & \Lambda_{65} & \Lambda_{66} & -5S_{26}a^2b^2 & -9S_{16}b^4 & -2S_{16} \\ -5S_{26}a^2 & 5S_{22}a^2 & 5S_{12}a^2 & \Lambda_{74} & -9S_{26}a^4 & -5S_{26}a^2b^2 & 9S_{22}a^4 & 5S_{12}a^2b^2 & S_{22} \\ -5S_{16}b^2 & 5S_{12}b^2 & 5S_{11}b^2 & \Lambda_{84} & -5S_{16}a^2b^2 & -9S_{16}b^4 & 5S_{12}a^2b^2 & 9S_{11}b^4 & S_{11} \\ 0 & 0 & 0 & \Lambda_{94} & -2S_{26} & -2S_{16} & S_{22} & S_{11} & 0 \end{bmatrix} \tag{33}$$

with

$$\begin{aligned} \Lambda_{14} &= -S_{16}a^2 - S_{26}b^2 & \Lambda_{24} &= S_{12}a^2 + S_{22}b^2 \\ \Lambda_{34} &= S_{11}a^2 + S_{12}b^2 & \Lambda_{41} &= -5S_{16}a^2 - 5S_{26}b^2 \\ \Lambda_{42} &= 5S_{12}a^2 + 5S_{22}b^2 & \Lambda_{43} &= 5S_{11}a^2 + 5S_{12}b^2 \\ \Lambda_{44} &= 9S_{11}a^4 + 9S_{22}b^4 + 10(S_{12} + 2S_{66})a^2b^2 & \Lambda_{45} &= -9S_{16}a^4 - 25S_{26}a^2b^2 \\ \Lambda_{46} &= -25S_{16}a^2b^2 - 9S_{26}b^4 & \Lambda_{47} &= 9S_{12}a^4 + 5S_{22}a^2b^2 \\ \Lambda_{48} &= 5S_{11}a^2b^2 + 9S_{12}b^4 & \Lambda_{49} &= 2S_{12} + S_{66} \\ \Lambda_{54} &= -9S_{16}a^4 - 25S_{26}a^2b^2 & \Lambda_{55} &= 9S_{66}a^4 + 20S_{22}a^2b^2 \\ \Lambda_{56} &= 5(4S_{12} + S_{66})a^2b^2 & \Lambda_{64} &= -25S_{16}a^2b^2 - 9S_{26}b^4 \\ \Lambda_{65} &= 5(4S_{12} + S_{66})a^2b^2 & \Lambda_{66} &= 20S_{11}a^2b^2 + 9S_{66}b^4 \\ \Lambda_{74} &= 9S_{12}a^4 + 5S_{22}a^2b^2 & \Lambda_{84} &= 5S_{11}a^2b^2 + 9S_{12}b^4 \\ \Lambda_{94} &= 2S_{12} + S_{66} \end{aligned}$$

References

[1] Ari-Pekka Honkanen and Simo Huotari. General procedure for calculating the elastic deformation and x-ray diffraction properties of toroidally and spherically bent crystal wafers. In preparation, 2020.

[2] Ari-Pekka Honkanen, Giulio Monaco, and Simo Huotari. A computationally efficient method to solve the takagi–taupin equations for a large deformed crystal. *Journal of Applied Crystallography*, 49(4):1284–1289, jul 2016. doi:10.1107/s1600576716010402.