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.

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[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

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

the corresponding strain tensor components

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

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

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

and the contact force per unit area

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

2.2.2 Anisotropic circular

The stretching stress tensor components are

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

where

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

the corresponding strain tensor

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

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

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

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

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

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

and the contact force per unit area

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

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

$$\sigma_{xx} = \frac{E}{gR_1 R_2} \left[\frac{a^2}{12} - x^2 + \left(\frac{1+\nu}{2} + 5\frac{a^2}{b^2} + \frac{1-\nu}{2}\frac{a^4}{b^4} \right) \left(\frac{b^2}{12} - y^2 \right) \right] \tag{15}$$

$$\sigma_{yy} = \frac{E}{gR_1 R_2} \left[\frac{b^2}{12} - y^2 + \left(\frac{1+\nu}{2} + 5\frac{b^2}{a^2} + \frac{1-\nu}{2}\frac{b^4}{a^4} \right) \left(\frac{a^2}{12} - x^2 \right) \right] \tag{16}$$

$$\sigma_{xy} = \frac{2E}{gR_1 R_2} xy, \tag{17}$$

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

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

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

$$\Lambda_{14} = -S_{16}a^2 - S_{26}b^2 \qquad\qquad \Lambda_{24} = S_{12}a^2 + S_{22}b^2$$

$$\Lambda_{34} = S_{11}a^2 + S_{12}b^2 \qquad\qquad \Lambda_{41} = -5S_{16}a^2 - 5S_{26}b^2$$

$$\Lambda_{42} = 5S_{12}a^2 + 5S_{22}b^2 \qquad\qquad \Lambda_{43} = 5S_{11}a^2 + 5S_{12}b^2$$

$$\Lambda_{44} = 9S_{11}a^4 + 9S_{22}b^4 + 10(S_{12} + 2S_{66})a^2b^2 \qquad\qquad \Lambda_{45} = -9S_{16}a^4 - 25S_{26}a^2b^2$$

$$\Lambda_{46} = -25S_{16}a^2b^2 - 9S_{26}b^4 \qquad\qquad \Lambda_{47} = 9S_{12}a^4 + 5S_{22}a^2b^2$$

$$\Lambda_{48} = 5S_{11}a^2b^2 + 9S_{12}b^4 \qquad\qquad \Lambda_{49} = 2S_{12} + S_{66}$$

$$\Lambda_{54} = -9S_{16}a^4 - 25S_{26}a^2b^2 \qquad\qquad \Lambda_{55} = 9S_{66}a^4 + 20S_{22}a^2b^2$$

$$\Lambda_{56} = 5(4S_{12} + S_{66})a^2b^2 \qquad\qquad \Lambda_{64} = -25S_{16}a^2b^2 - 9S_{26}b^4$$

$$\Lambda_{65} = 5(4S_{12} + S_{66})a^2b^2 \qquad\qquad \Lambda_{66} = 20S_{11}a^2b^2 + 9S_{66}b^4$$

$$\Lambda_{74} = 9S_{12}a^4 + 5S_{22}a^2b^2 \qquad\qquad \Lambda_{84} = 5S_{11}a^2b^2 + 9S_{12}b^4$$

$$\Lambda_{94} = 2S_{12} + S_{66}$$

2.2.5 Tensors in cylindrical coordinates

Internally TBCALC performs the computations in the Cartesian coordinates (x, y, z) but especially with the circular analysers expressing the strain and stress tensors in the cylindrical system (r, ϕ, z) can be useful. The implemented coordinate transform `cartesian_tensors_to_cylindrical` uses the

following formula

$$T'_{rr} = \cos^2\phi\, T_{xx} + 2\sin\phi\cos\phi\, T_{xy} + \sin^2\phi\, T_{yy} \tag{34}$$

$$T'_{r\phi} = -\sin\phi\cos\phi\, T_{xx} + (\cos^2\phi - \sin^2\phi) T_{xy} + \sin\phi\cos\phi\, T_{yy} \tag{35}$$

$$T'_{\phi\phi} = \sin^2\phi\, T_{xx} - 2\sin\phi\cos\phi\, T_{xy} + \cos^2\phi\, T_{yy} \tag{36}$$

$$T'_{rz} = \cos\phi\, T_{xz} + \sin\phi\, T_{yz} \tag{37}$$

$$T'_{\phi z} = -\sin\phi\, T_{xz} + \cos\phi\, T_{yz} \tag{38}$$

$$T'_{zz} = T_{zz}. \tag{39}$$

Strictly speaking ϕ is actually handled here as $r\phi$ in order to keep the physical unit of the coordinates and thus the dimensions of the transformed tensor components consistent with the Cartesian representation.

2.3 Energy and angle shifts due to transverse deformation

Locally the shape of the reflection curve is given by the 1D TT-curve but its position on the energy or angle scale is shifted by the transverse deformations given in Section 2.2. When the energy is scanned the shifts are given by

$$\frac{\Delta\mathcal{E}}{\mathcal{E}} = -u_{zz}\cos^2\phi - 2u_{xz}\sin\phi\cos\phi - u_{xx}\sin^2\phi + \left[(u_{zz} - u_{xx})\sin\phi\cos\phi + 2u_{xz}\sin^2\phi\right]\cot\theta_B \quad (40)$$

where θ_B is the Bragg angle and ϕ is the asymmetry angle. Similarly in the rocking angle scan the shifts in angle are given by

$$\Delta\theta = -\left(u_{zz}\cos^2\phi + 2u_{xz}\sin\phi\cos\phi + u_{xx}\sin^2\phi\right)\tan\theta_B + (u_{zz} - u_{xx})\sin\phi\cos\phi + 2u_{xz}\sin^2\phi. \quad (41)$$

2.4 Johann error

The shifts in the angle due to Johann error are

$$\Delta\theta = \frac{x^2}{2R_1^2}\cot\theta - \frac{(R_1 - R_2)(R_1\sin^2\theta - R_2)}{2R_1 R_2 \sin\theta\cos\theta}y^2 \tag{42}$$

and in terms of energy

$$\Delta\mathcal{E} = -\frac{x^2}{2R_1^2}\mathcal{E}\cot^2\theta + \frac{(R_1 - R_2)(R_1\sin^2\theta - R_2)}{2R_1 R_2 \sin^2\theta}\mathcal{E}y^2. \tag{43}$$

Note that the expression for $\Delta\theta$ is derived expanding $\sin x$ to the first order and thus ceases to be valid near $\theta = \pi/2$ if $R_1 \neq R_2$.

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.