

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 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 matrices¹ are used for elastic parameters and XRAYLIB² for crystallographic parameters and structure factors.

¹Values 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 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

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

the corresponding strain tensor components

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

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

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

and the contact force per unit area

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

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.