TBCALC: The Technical Document
Version 1.0

Ari-Pekka Honkanen

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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`

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.