Diffraction Anomalous Fine Structure in Laue Geometry:
First Tests on LiTaO$_3$

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The method of Diffraction Anomalous Fine Structure (DAFS) combines the long-range sensitivity of diffraction with the short-range sensitivity of XAFS by measuring the intensity of a reflection at different energies around the corresponding absorption edge. The aim of the analysis is to find a Kramers-Kronig related pair of $f'(E)$ and $f''(E)$ that fits to the measured intensity. The use of the Kramers-Kronig transformation limits the method to centrosymmetric crystals. Our aim is to overcome this restriction by measuring a reflection in Laue and in Bragg geometry. The intensity measured in Laue geometry contains additional information about the structure factor $F_H$ [1]. This can be used to extract $f'(E)$ and $f''(E)$ by comparison of the intensity in Bragg and Laue geometry. As no Kramers-Kronig transformation is applied in this approach, it could be utilised to non-centrosymmetric systems, too.

The first steps in this direction are the measurement of centrosymmetric reflections in Laue geometry and comparison with standard XAFS.

In the following the analysis of the $\bar{1}20$ reflection of Lithium Tantalate (LiTaO$_3$) will be described. Lithium Tantalate has been chosen as system due to its well known, trigonal structure with a polar c-axis.

In order to obtain the fine-structure function $\chi''_w$ from the measured intensity it is necessary to separate $|F_H|$ into the smooth and the oscillatory part.

After fitting the intensity using Cromer-Liberman values, $f''_w$ can be obtained by means of a Kramers-Kronig transformation of $(f'_a - f'_w)$ [2]

$$f''_w(E) = f''_a - \frac{2E}{\pi} P \int_{\Delta E} \frac{f''_0(E')\chi'_w(E')}{E'^2 - E^2} dE'.$$

(Figure 1 (top left) compares the measured and modeled intensity. The mismatch at the white line is caused by the fact, that the absorption of the sample is so high, that no photons are transmitted at the white line energy. This causes the big peak in $f'_w$ (Figure 1 (top right)) and the dip before the edge in $f''_w$ (Figure 1 (bottom left)). Figure 1 (bottom right) compares the $k\chi(k)$ extracted from a XAS spectrum of a LiTaO$_3$ powder pellet (black) and from $f''_w$ (blue). An EXAFS analysis with standard tools is in progress.

References

Figure 1: Top left: Measured DAFS signal of the (120) Laue reflection (blue) and modeled intensity (black). Top right: Final $f_{\text{w}'}$ (blue) compared to Cromer-Liberman calculated $f_{\text{a}'}$ (black). Bottom left: Final $f_{\text{w}''}$ (blue) and Cromer-Liberman calculated $f_{\text{a}''}$ (black). Bottom right: $k\chi(k)$ extracted from the XAS spectrum of the LiTaO$_3$ powder pellet (black) and from $f_{\text{w}''}$ (blue).