ESRF	**Experiment title:** Anisotropy in Borrmann Spectroscopy at Phase Transitions	**Experiment number:** HE-3958
Beamline: BM28	**Date of experiment:** from: 07 Nov 2012 to: 13 Nov 2012	**Date of report:**
Shifts: 18	**Local contact(s):** Didier Wermeille	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):
T. Laurus[1,*], M. Tolkiehn[1,*], S. P. Collins[2,*], L. A. Martín-Montoya[3,*]

[1]FS-DO, DESY, Notkestraße 85, 22603 Hamburg, Germany
[2]Diamond Light Source Ltd, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom
[3]Department Chemie, Fakultät für Naturwissenschaften, Universität Paderborn, Warburger Straße 100, 33098 Paderborn, Germany

Report:
In recent publications [1,2] we have developed a framework for the description of the quadrupole enhancement and its dependence on temperature and electronic anisotropy. The goal of this experiment was the extension of this framework to phase transitions. Therefore, we studied the temperature dependence of the quadrupole enhancement of barium titanate (BTO) whithin the range of 15 - 300 K. Figure 1 shows the normalized absorption of BTO (110) reflection at quadrupole resonance (4.970 keV), the main absorption maximum (4.986 keV) and an energy above the Ti K edge (5.02 keV) for the rhombohedral-to-orthorhombic and the orthorombic-to-tetragonal phase transitions. Due to problems with the used temperature controller the temperature resolution around the phase transitions was not sufficient.
In the second part of the experiment we performed diffraction anomalous fine structure experiments in Bragg and Laue geometry at BTO. Figure 2 (Left) shows the measured intensity of the $(10\bar{1})$ (Bragg) and $(0\bar{1}1)$ reflection (Laue). The Bragg and Laue spectra contain different fine structure, which is visible in Figure 2 (Right). Conventional DAFS (only Bragg geometry) is restricted to centrosymmetric crystals due to the use of Kramers-Kronig transformations. The Laue geometry reflectivity contains additional information, that will be utilized in an ongoing analysis for the extraction of the fine structure function. This approach extends the method of DAFS to non-centrosymmetric systems.

In the last part of the experiment we performed first multiple beam diffraction anomalous fine structure experiments [3] in Laue geometry at BTO. They consisted of Renninger scans (Figure 3 (Left)) of the $\bar{1}10$ reflection at energies around the Ti K edge. The absorption spectrum extracted from the Renninger scans is shown in Figure 3 (Right).

We acknowledge the extensive support by the BM28 staff during our beamtime.

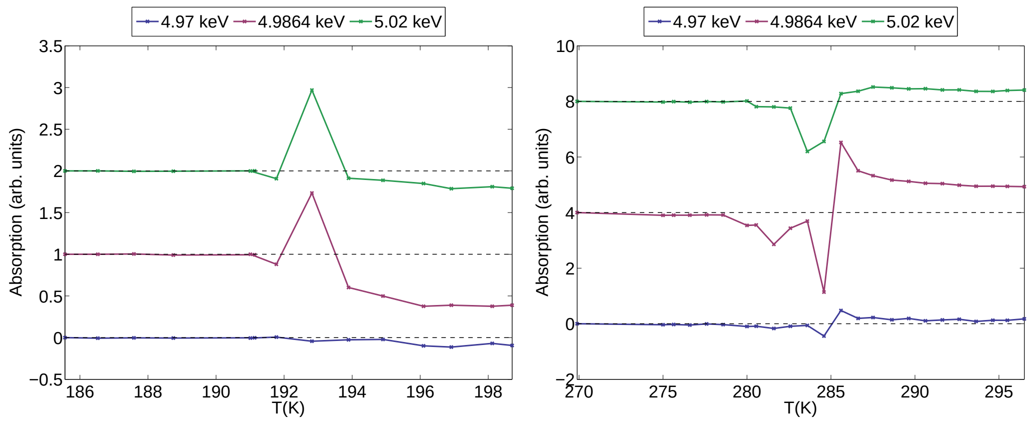

Figure 1: Comparison of the normalized absorption at BTO (110) reflection at quadrupole resonance (4.970 keV), the main absorption maximum (4.986 keV) and an energy above the Ti K edge (5.02 keV) for the rhombohedral-to-orthorhombic (Left) and the orthorombic-to-tetragonal (Right) phase transition. For clarity, the curves are shifted by a multiple of 1 and 4 respectively.

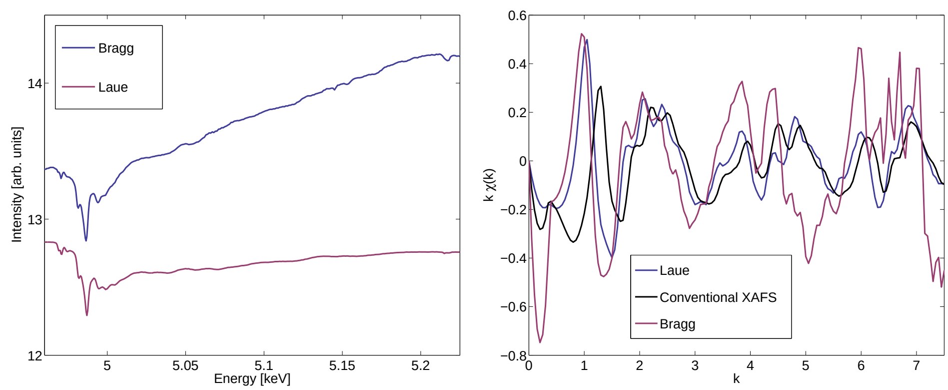

Figure 2: Left: Diffraction Anomalous Fine Structure spectra of $(10\bar{1})$ (Bragg) and $(0\bar{1}1)$(Laue). Right: Fine structure extracted from Bragg and Laue spectra compared to conventional XAFS.

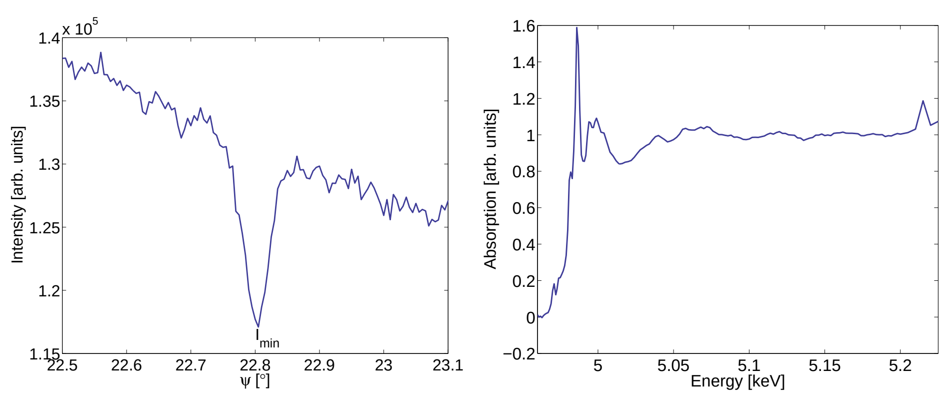

Figure 3: Left: Renninger scan of $(\bar{1}10)$ reflection at 5 keV. Right: Absorption spectrum extracted from the Renninger scans.

[1] M. Tolkiehn, T. Laurus, and S. P. Collins Phys. Rev. B **84**, 241101(R) (2011)

[2] M. Tolkiehn, T. Laurus, and S. P. Collins, Phys. Rev. B in prep.

[3] Y.-R. Lee et al., Phys. Rev. Lett. **97**, 185502 (2006)