Borrmann Spectroscopy of Fe-doped SrTiO$_3$

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The Borrmann effect describes a dramatic increase in transmission at certain Laue reflections for X-rays [1]. This is caused by the standing wave field in the crystal. The electric field amplitude is close to zero at the atomic sites, which leads to a vastly decreased dipole absorption [2]. At the same time the electric field gradient is maximized, which causes a strong relative enhancement of quadrupole absorption [3, 4].

We used this effect to study the pre-edge structure of SrTiO$_3$ doped with 0.13 wt % iron at the Ti-K edge. The sample had a dimension of 10 x 10 x 0.5 mm$^3$. The experiment was performed at P09 at PETRA III, HASYLAB. The integrated intensities of the (002) and (011) reflections were measured for different energies around the Ti-K edge by detecting the Laue-diffracted beam, and the fluorescence yield measured under the same conditions, using a Vortex silicon drift detector. The purpose of the measurements was look for an increase in any of the pre-edge peaks due to the enhanced quadrupole sensitivity in the Borrmann effect, and to determine the temperature dependence of the dipole and quadrupole features. The latter was achieved using a closed cycle Displex cryostat.

A huge enhancement of the first pre-edge peaks is very clearly evident, even in the raw data, which confirms it’s origin as predominantly quadrupole, in agreement with DFT calculations [5]. Figure 1 shows the Ti-K edge fluorescence absorption spectrum and the (002) Borrmann spectrum of Fe-doped SrTiO$_3$. Both spectra are background subtracted and normalized to the edge-jump.

![Figure 1](image)

Figure 1: Absorption of Fe-doped SrTiO$_3$ at the Ti-K edge determined from fluorescence yield (blue line) and from the intensity of the (002) Laue reflection (red line).

Figure 2 shows the (002) Borrmann spectra of Fe-doped SrTiO$_3$ for 6 K and 310 K. The intensity of the first pre-edge peak does not change with temperature while the rest of the spectrum increases, which is in qualitative agreement with the first peak being a Borrmann-enhanced quadrupole peak. A detailed analysis is in progress.
Figure 2: Comparison of the Ti-K edge Borrmann spectra of Fe-doped SrTiO$_3$ for 6 K and 310 K.

References