ESRF	**Experiment title:** Quadrupolar transitions in x-ray absorption	**Experiment number:** HE-533
Beamline: ID12A	**Date of experiment:** from: Feb 5, 1999 to: Feb 11, 1999	**Date of report:** Jul 27, 1999
Shifts: 18	**Local contact(s):** A. Rogalev, J. Goulon	*Received at ESRF:* 23 AOUT 1999

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Report:

The angular dependence of the x-ray absorption spectra of cubic crystals is a unique method to determine the position and intensities of quadrupole transitions. Last year, we performed a careful experimental investigation of the angular dependence of x-ray absorption spectra at the K-edge of iron in pyrite. These experiments are now analyzed from three points of views: multiple-scattering theory, non-muffin-tin theory, multiplet theory [1]. The first two are one-electron theories and give too small a signal as compared to experiment, the multiplet approach is essentially atomic and yields too large a signal. A measurement of the intensity of quadrupole transitions is important to estimate the quadrupole contribution to magnetic circular dichroism. An experimental intensity intermediate between a localized and a delocalized models is natural, since the d electrons of Fe in pyrite are rather strongly hybridized with their sulphur neighbours.

To check this measurement of intensity, it was interesting to investigate the quadrupole transitions at the K-edge of titanium, where one-electron and atomic models should give essentially the same result. Only two samples were measured during the available shifts, because the experience of pyrite taught us that a detailed angular dependence must be measured at each energy point. This is the only way to discard the strong artefacts due to diffraction peaks of the single-crystal sample. Therefore spectra are measured at 120 angles and 500 energies, which makes 60000 data that are analyzed to get one spectrum. A first series of experiments (see fig.1) have been carried out successfully at the K-edge of titanium in $SrTiO_3$. This crystal is cubic and was cut perpendicular to the [110] direction to obtain a maximum intensity of the angular dependence.

A clear and clean signal was obtained in the region of the pre-edge peaks, together with a small contribution at higher energy. These results do not agree with a strict atomic point of view, and the multiple-scattering and the non-muffin-tin approaches will be tested on this case. The second series of experiments have been carried out equally successfully at the K-edge of titanium in $BaTiO_3$. Again, a very clean and reproducible signal was obtained at different points of the sample. This crystal is quadratic, and the signal is much larger than in $SrTiO_3$. The reason for such a large signal is not yet clear. It could be due to a contamination by electric dipole signal due to the fact that the sample was not perfectly oriented, or it could be a genuine effect. Again, the experimental results will be compared with calculations.
We would like to conclude by stressing that the beamline has worked excellently during all the shifts, with very stable and reproducible results.

Reference

Ch. Brouder, D. Cabaret, M.-A. Arrio, J. Goulon, Ch. Goulon-Ginet, A. Rogalev and Y. Joly, *Angular dependence of x-ray absorption in cubic crystal: the case of pyrite*, in preparation

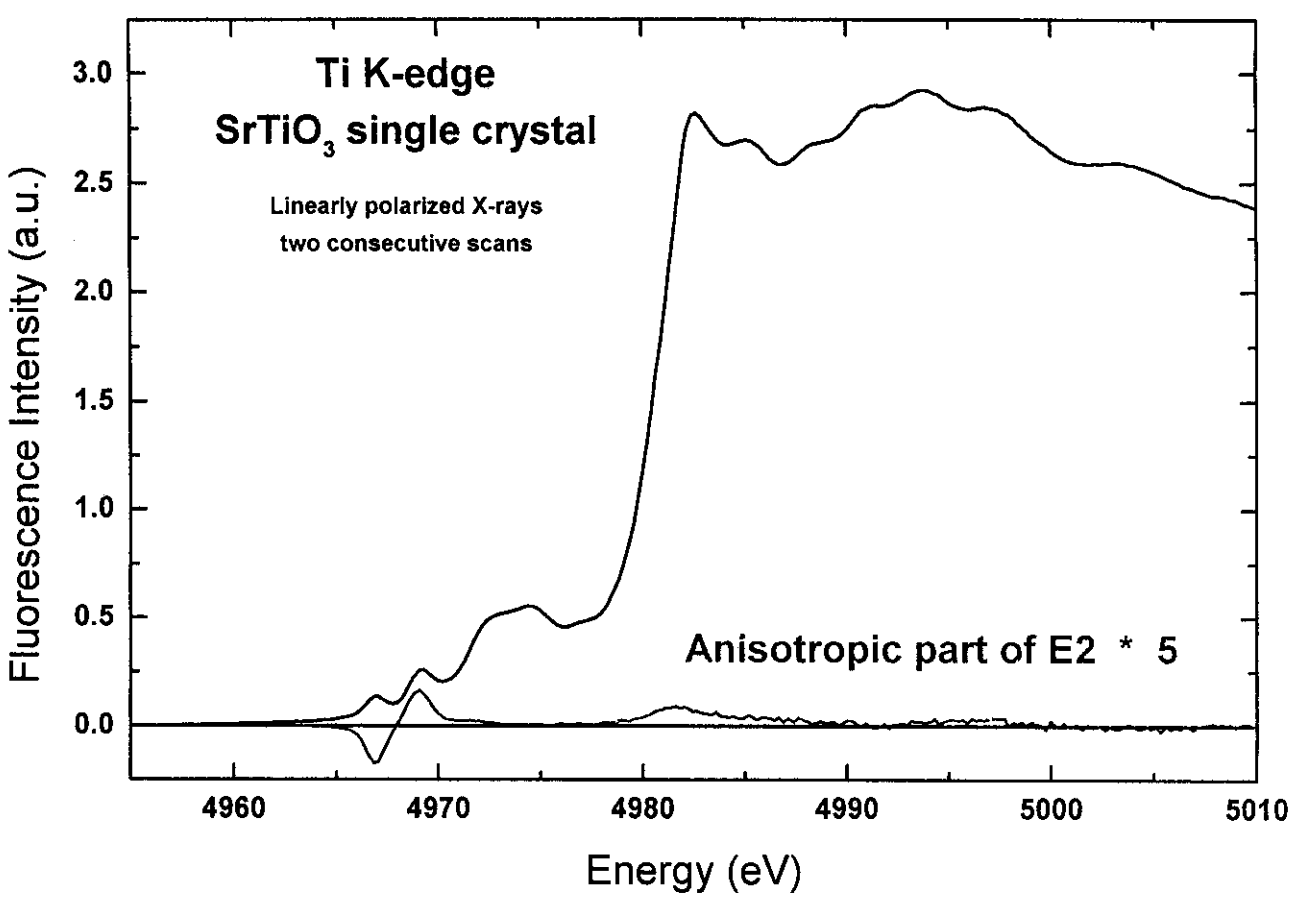

Fig.1. X-ray absorption spectra and angular dependence at the K-edge of titanium in $SrTiO_3$.