ESRF	**Experiment title:** Three dimensional imaging of dopant atoms in non perfect crystals with kinematical X-ray standing waves	**Experiment number:** HS-2937
Beamline: ID32	**Date of experiment:** from: September 21, 2005 to: September 27, 2005	**Date of report:** June 27, 2006
Shifts: 18	**Local contact(s):** Tien-Lin Lee	*Received at ESRF:*

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Report:
The aim of our experiment was to determine the three dimensional position of the La and Sr atoms in a mosaic $LaSrMnO_4$ single crystal.
$LaSrMnO_4$ has perovskite structure, with La and Sr atoms occupying the same position in the unit cell. Up to now, only the average position of the La and Sr atoms is known, and it appeared to be impossible to determine the positions separately by common methods. In our experiment, we have used the novel kinematical x-ray standing waves (KXSW) method to solve this problem.
The experiment was split into two parts. First, we performed KXSW measurements at different Bragg reflections at 6.6 keV. As secondary signal we recorded the Sr L, La L and Mn K fluorescence.
In the second part of the experiment we measured the secondary signal within a large solid angle similar to multiple energy x-ray holography (MEXH). For this type of measurement, we designed a specialized apparatus in consideration of the ID32 beam parameters and available equipment. The device consists of a double circle spectrometer, fast data acquisition and control electronics and custom-made software. The spectrometer combines a standard Huber 410 rotation stage with a fast servo motor driven rotation axis. During the experiment the fast axis rotates continuously at a constant speed of up to 120 rpm. The slower Huber axis can be moved either in incremental steps or continuously and synchronized with the fast axis.

Results:

A typical KXSW curve measured in the first part of the experiment is shown in figure 1. Since the position of the Mn atoms are known, the Mn K fluorescence was used as a reference. Besides, it allowed us to determine the reduction of the coherent fraction caused by the imperfectness of the lattice. The La L fluorescence yield was then used to determine the distance between the La and Mn atoms. The obtained value of $d_{La} = 4.59 \pm 0.05$Å deviates from the average La/Sr position. The Sr position could not be obtained directly from the experimental results due to the small Sr L absorption cross-section at the used incident beam energy and the low counting statistics of the Sr data. Therefore, the Sr atom position was determined indirectly from the known average position to be $d_{Sr} = 4.79 \pm 0.05$Å.

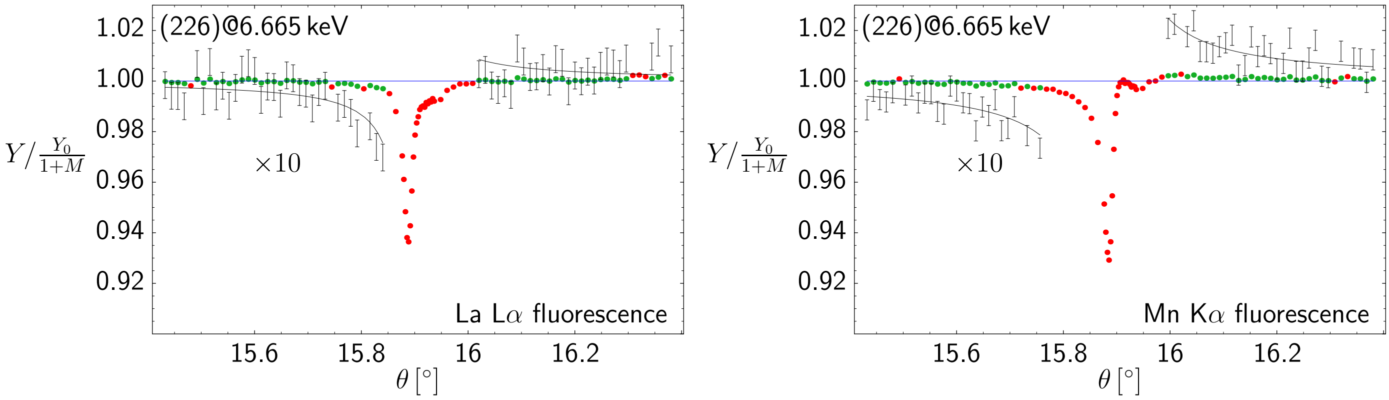

Figure 1: La and Mn fluorescence yield, the red dots are data points excluded from evaluation, the green dots are also shown magnified with error bars and the best fit (solid line)

In the second part of the experiment we measured the La fluorescence in a large solid angle region (figure 2). Unfortunately, the stability of the old ID32 monochromator appeared to be not sufficient for that type of measurements: the fast and random variations of the incident beam intensity can not be reliably removed from the measured curves. Therefore, we had to exclude a significant amount of data from further analysis, ending up with data sets containing statistic too low for quantitative evaluation with required level of precision. However, it is clear, that the divergence and intensity of the beam are sufficient for the experimental method we have used.

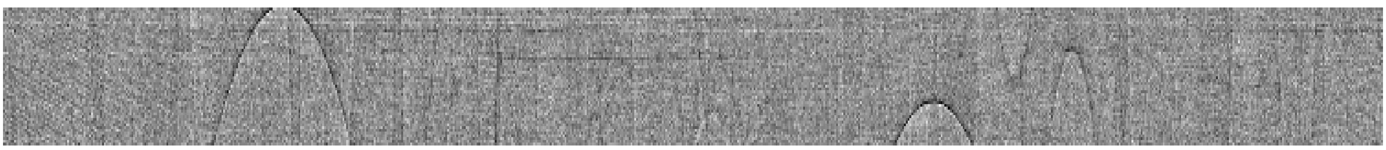

Figure 2: La fluorescence measured in a 2° by 360° solid angle region

Prospects:

During our beam time we have for the first time applied a novel experimental method to real samples. Our new apparatus specially designed for that experiment proved to be effective and well compatible with the ID32 equipment. The obtained results have provided new information on crystalline structure of $LaSrMnO_4$. We are currently preparing the publication of the of the results.

We acknowledge the extensive support by Dr. T.-L. Lee and Dr. J. Zegenhagen during our beamtime and the very user friendly operation rules and procedures at the ID32 beamline.