ESRF	**Experiment title: Charge ordering in the manganite system $CaMn_7O_{12}$ studied by anomalous diffraction**	**Experiment number**: HE 1528
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Shifts: 9	**Local contact(s)**: A. Fitch	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

R. Przeniosło(*), A. Palewicz(*), I. Sosnowska

Institute of Experimental Physics, Warsaw University

E. Suard (ILL)

Report:

Earlier studies of $CaMn_7O_{12}$ by neutron diffraction and non-resonant SR diffraction have shown a crystallographic phase transition in which the trigonal and cubic phases coexist in a temperature interval from 410 K up to 450 K [1,2]. The analysis of the Jahn-Teller effect of the $Mn^{3+}O_6$ octahedra [1,2] was in agreement with the conjecture [3] that the trigonal phase is charge ordered and the cubic phase is charge delocalized. In order to verify this interpretation we have performed studies of the crystallographic phase transition in $CaMn_7O_{12}$ by diffraction at anomalous fine structure (DAFS) at the ID31 beamline.

The SR diffraction patterns of $CaMn_7O_{12}$ were measured at several X-ray energies around the Mn^{3+} and Mn^{4+} absorption K edges. The measurements have been performed in the Q-range $0.7\ Å^{-1} < Q < 5.7\ Å^{-1}$. The fluorescence intensity was measured with an additional detector.

Selected SR diffraction patterns of $CaMn_7O_{12}$ in the trigonal, charge ordered phase measured for several X-ray energies around the Mn^{3+} and Mn^{4+} absorption K edges are shown in Fig. 1. One can see that the intensity ratios of the Bragg diffraction peaks change with X-ray energy. These changes can be explained by assuming that Mn^{3+} and Mn^{4+} ions

occupy different crystallographic positions and their X-ray scattering contributions change with X-ray energy.

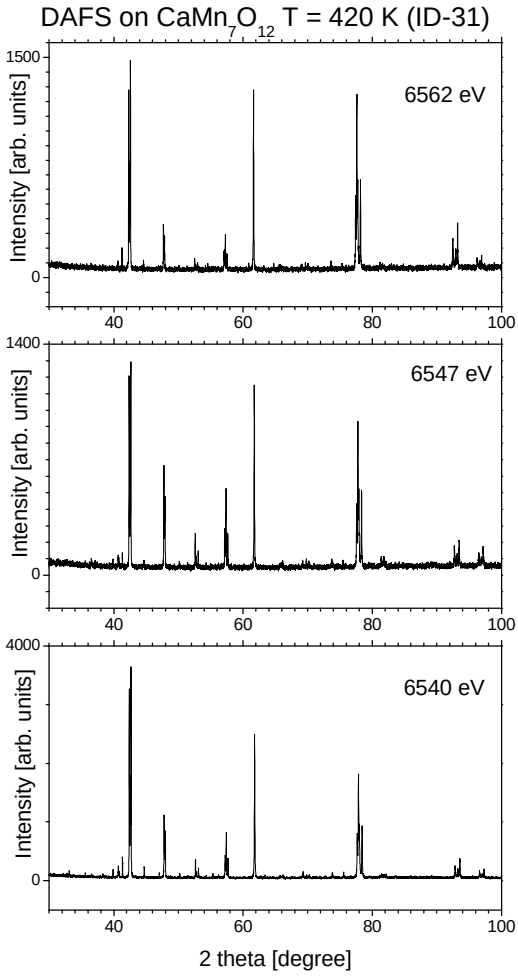

Fig. 1. SR powder diffraction patterns of $CaMn_7O_{12}$ measured at different X-ray energies close to the Mn^{3+}/Mn^{4+} absorption edges. These measurements were done at T = 420 K where the majority of the sample volume is in the low temperature trigonal phase [1].

The diffraction patterns measured at higher temperatures, where the two crystallographic phases coexist show a similar behaviour. The main goal of further data analysis is to obtain information about the distribution of Mn^{3+} and Mn^{4+} ions within the phase transition range.

References

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[2] R. Przeniosło, W. Van Beek and I. Sosnowska, Solid State Communications **126** (2003) 485.

[3] B.Bochu, J.L.Buevoz, J.Chenavas, A.Collomb, J.C.Joubert and M.Marezio, Solid State Commun. **36** (1980) 133.