ESRF	**Experiment title: Study of the changes of the crystal structure of $CaMn_7O_{12}$ at magnetic phase transitions**	**Experiment number**: HE-896
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Report:

The main goal of this experiment was to verify whether the magnetic phase transitions observed at 49 K and 90 K in $CaMn_7O_{12}$ [1-3] are associated with changes of the crystal structure and/or possibly by charge and orbital ordering. Another part of this experiment was devoted to a study of the trigonal to cubic crystallographic phase transition observed at 450K in $CaMn_7O_{12}$ which was briefly described in [4].

The SR powder diffraction measurements of $CaMn_7O_{12}$ have been performed at a wavelength of 0.71029 Å for several temperature steps between 10 K and 450 K. The resulting SR diffraction patterns were analysed by the Rietveld method by using the program FullProf [5]. The diffraction patterns observed below 400 K can be refined with the use of the trigonal space group $R\bar{3}$ and the starting structural model given in [6]. The resulting values of the lattice parameters (in hexagonal setting) and the unit cell volume are shown in Figs. 1 (a) and (b). One can conclude that in the vicinity of the magnetic phase transitions, i.e. at 49 K and 90 K there are no considerable changes of the lattice constants. One can see the contraction of the lattice constant in the c-direction with a minimum near 250 K which indicates that the thermal lattice expansion is highly anisotropic. The decrease of the c parameter between 50 K and 250 K is

compensated by the increase of the a parameter, so the unit cell volume is increasing with temperature.

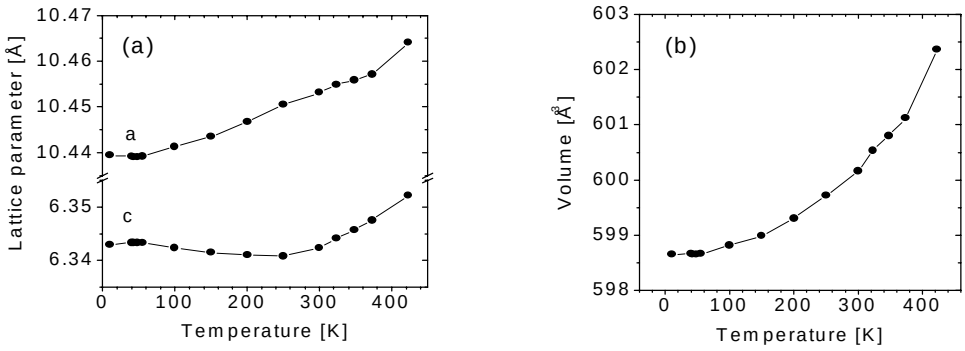

Fig.1 Temperature dependence of the lattice parameters (a) and unit cell volume (b) of $CaMn_7O_{12}$ in the trigonal phase. The lattice parameters are given in the hexagonal setting.

There are three weak reflections which can be due to a charge ordering in $CaMn_7O_{12}$. Their intensity gradually decrease with temperature and finally vanish at 250 K. Two of them match within less than $5*10^{-4}$ relative error to the (210) and (310) reflections which are forbidden in the trigonal crystal structure of $CaMn_7O_{12}$ [6]. Neutron diffraction studies showed that the ferrimagnetic ordering in $CaMn_7O_{12}$ (below 90 K) [2] contributes to magnetic Bragg peaks at (210) and (310) what suggests that the charge and magnetic orderings in $CaMn_7O_{12}$ are related to each other.

Measurements performed between RT and 450 K have shown interesting properties of the crystallographic phase transition. Up to 383 K there are only Bragg peaks which are due to the trigonal phase. Above 403 K the Bragg peaks due to the cubic phase (space group $Im\bar{3}$) appear and their intensity increases with temperature. The intensity of the Bragg peaks due to the trigonal phase decrease with temperature and goes to zero at 443 K. It is interesting to note that in the 40 K wide interval between 403K and 443K both phases coexist, and both correspond to a long range ordering, since all the Bragg peaks have similar widths.

References

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