ESRF	**Experiment title:** Structural P-T phase diagram of $EuTiO_3$	**Experiment number**: HC-1913
Beamline: ID27	**Date of experiment**: from: 02/03/2015 to: 07/03/2015	**Date of report**: 09/07/2015
Shifts: 11	**Local contact(s)**: Paraskevas PARISIADIS	*Received at ESRF:*
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Report:

The goal during this allocated beamtime was to study the structural P-T phase diagram of multiferroic $EuTiO_3$ using x-ray powder diffraction. Low temperature data at ambient pressure for this material show a cubic-to-tetragonal phase transition with a critical temperature ranging from 160 to 285 K [1-4], depending on the technique used and the quality of the samples. High pressure structural data do not exist in the bibliography, however, as written in the proposal we suspect that there is a similar structural transition with pressure, as with temperature.

During the experiment on ID27 we indeed verified the transition under pressure. We performed measurements on a total of 5 diamond anvil cells, with pressure runs up to 50 GPa at constant temperatures 50, 200, 300, 400, and 500 K, including a detailed collection on cooling from 300 to 10 K, under a constant pressure of ~1.1 GPa. An example is shown in Figs.1&2 for low and high temperature data, where a clear splitting for the majority of peaks occurs under pressure, while a few peaks, as the (hhh) family, remain unperturbed. By indexing the structure we found a transition from the cubic *Pm-3m* to the tetragonal *I4/mcm* structure, as in the reported low temperature datasets.

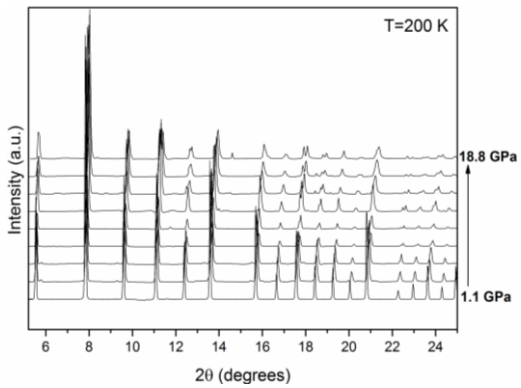

Fig.1 High pressure run at 200 K for $EuTiO_3$.

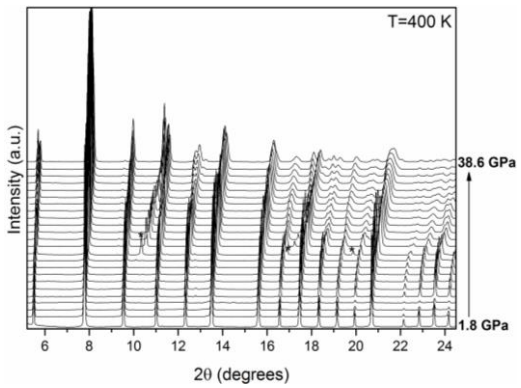

Fig.2 High pressure run at 400 K for $EuTiO_3$.

This transition is due to the rotational instability of TiO_6 octahedra which is common for ABO_3 perovskites and can be generated by a Jahn-Teller effect. It is interesting that the same transition occurs in the isostructural $SrTiO_3$ as well, although at a much lower temperature, due to the absence of multiferroic behavior in this compound [5]. The transition has been observed in all the 5 different datasets, as well as on cooling. The increase in the FWHM of the (200) peak has been defined as the parameter of the transition, and some examples of the refinement can be seen in Figs.3a&b.

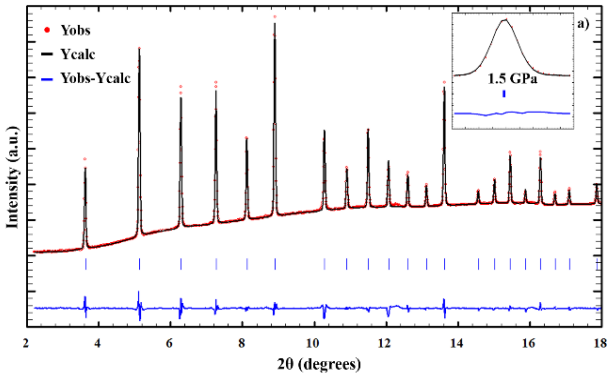

Fig.3a Lebail refinement of the tetragonal structure at 1.5 GPa. In the inset the (200) reflection is shown.

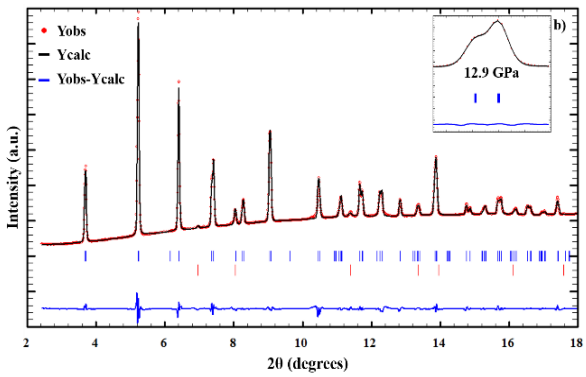

Fig.3b Lebail refinement of the tetragonal structure at 12.9 GPa. In the inset the (200) reflection is shown.

The large number of measurements at different temperatures allowed us to make a good estimation of the transition boundaries in temperature and pressure. Therefore, as a final outcome of this study we managed to establish a first structural phase diagram for $EuTiO_3$. The data can be fitted by a straight line that separates the cubic and tetragonal structures, as in the case of $SrTiO_3$ [5]. The linear fit yields a transition temperature of ~220 K at ambient pressure. It has been proposed that the large scattering of the data for the transition temperature are due to the existence of local tetragonal regions inside a long-range cubic phase [3]. The results of this proposal are published online at arXiv:1505.05049 and a paper has already been submitted to Phys. Rev. B.

References

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