ESRF	**Experiment title:** Structure determination in the perovskite $PbFe_{0.5}Ta_{0.5}O_3$ performed by synchrotron radiation powder diffraction.	**Experiment number**: CH-511
Beamline: BM16	**Date of experiment**: from: 8/7/98 to: 11/7/98	**Date of report**: 22/02/99
Shifts: 9	**Local contact(s)**: Eric DOORYHEE	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Sciau Phillippe CEMES-CNRS, BP 4347, 31055 Toulouse Cedex

Lampis Nathascia, Dipart. di Scienze Fisiche dell'Università e INFM,
Via Ospedale 72, 09124 Cagliari (Italie)

Geddo-Lehmann Alessandra, Dipart. di Scienze Fisiche dell'Università e INFM,
Via Ospedale 72, 09124 Cagliari (Italie)

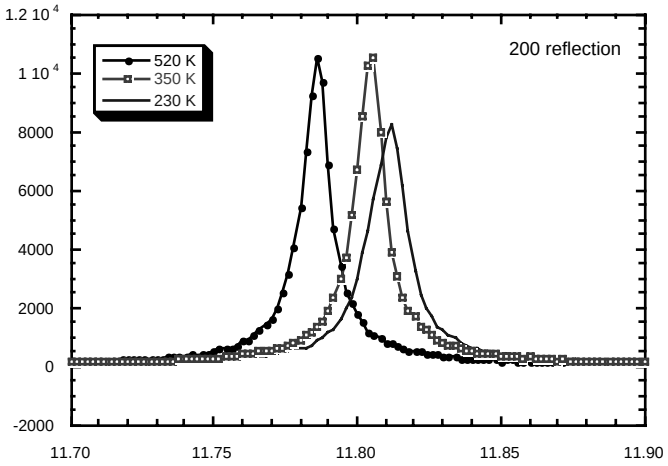
Report:

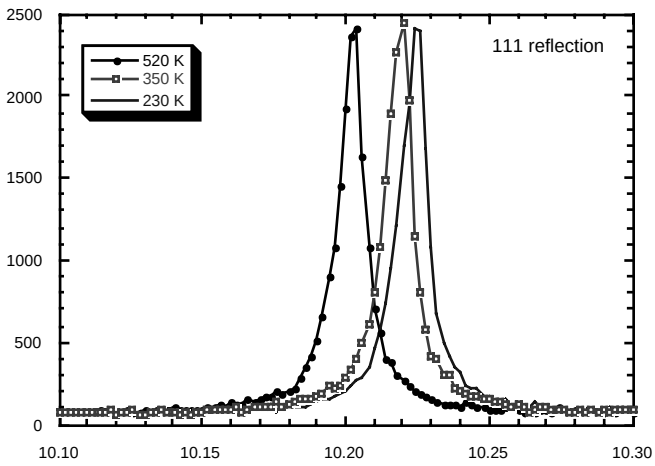
$PbFe_{0.5}Ta_{0.5}O_3$ belongs to the wide family of lead-based perovskites with general formula $PbB'_{0.5}B''_{0.5}O_3$. Materials of this kind typically undergo a sequence of temperature-induced ferroic phase transitions, which from the structural point of view consist in small distortions of a highly symmetric *parent phase* or *prototype.* The simple sequence of phases one still finds in Landolt-Boernstein [new series 1990 group III, vol. 28 (Berlin, Springer)], according to which this compound would belong to the ferroic specie $m\bar{3}mF3m$ - in the Aizu notation - has been put under discussion since single crystals were synthesized. Earlier observations supported the existence of *two* phase transitions and the rhombohedral symmetry of the lowest temperature phase is still questionable. The presence of two transitions has recently been confirmed by high resolution X-Ray diffraction and polarized light microscopy both performed on single crystals [A. Geddo Lehmann, Ph. Sciau, J. Condens Matter, to be published]. The transition temperatures were measured as 270 K and 200 -220 K. The ferroelastic domain structure is very complex in the low temperature phases and makes difficult the structural determination from single crystal.
Five complete patterns were collected at 15K, 130K, 230K, 350K and 520K on BM16 (λ=0.41 Å). The study of the distortion vs temperature of the low phases has not been done by lack of time. In the cryostat, the background was very important and

several shifts were necessary for to determine the origin of the diffusion and find the good conditions to collect the diffraction patterns.

The structure at 520K and 350K is cubic (Pm3m). However analysis of the structure factor $|F|$ reveals the noticeable nonmonotony of $|F|$ vs $\sin\theta/\lambda$. This nonmotony may be caused by differences of the atomic form factors, anharmonicity of thermal motion nd atomic displacements. In our case, the possible reasons are atomic disorder and anharmonic thermal motion. The effect is more pronounced at 350 K.

At 230K no splitting of reflections is observed but a significant increase of the full width at half maximum (FWHM) of h00 reflections is observed. On the contrary the hhh reflections do not show a significant evolution. These results are consistent with the tetragonal symmetry proposed in the study on single crystals. A fit of the complete diffraction patterns give : a=4.0067(3)Å c=4.0085(5)Å. The c value is very close to the one obtained on single crystal (c=4.0086 Å). From these data, we tried to fit the neutron powder diffraction patterns to obtain the structure.





At 130K and 15 K, The splitting of the hhh reflections is observed but the h00 reflections remain wide. The real symmetry seems to be monoclinic. A structural determination both by X-ray and neutrons powder diffraction is in progress.