



	<b>Experiment title:</b> <b>Surface and Interface Structural determination in highly ordered strained BFO islands</b>	<b>Experiment number:</b> HC-4563
<b>Beamline:</b>	<b>Date of experiment:</b> from: 15/09/2021 to: 20/09/2021	<b>Date of report:</b> 24/03/2021
<b>Shifts:</b>	<b>Local contact(s):</b> Maurizio De-Santis	<i>Received at ESRF:</i>
<b>Names and affiliations of applicants</b> (* indicates experimentalists): Adrian Crespo villanueva, ICMAB-CSIC (SPAIN) Dr. Maurizio De Santis, Institut Neel, CNRS, Grenoble (FRANCE) Dr. Veronique Langlais Abad, CEMES-CNRS, Toulouse (FRANCE) Dr. Javier Torrelles albareda, ICMAB-CSIC (SPAIN)		

## Report:

The BiFeO<sub>3</sub> system shows different magnetic and electric behaviors associated to the structural quality and dimensionality of epitaxial films and islands under misfit strains induced by the substrate. In nanoscale islands, size, shape and strain effects sum up to control the topological distribution of ferroelectric (FE) domains and the properties of the domain walls separating them. The recent synthesis of BFO islands epitaxially grown on SrTiO<sub>3</sub>(001) by PLD in our lab at nearly “single crystal” quality, offers the opportunity to study the intrinsic structure of these islands as well as that of their surface.

In order to understand the intrinsic properties of this system we have studied the surface structure of these islands as well as its average inner structure by means of surface x-ray diffraction at BM32 beamline.

Several BiFeO<sub>3</sub>(001) epitaxial films (25 and 50 nm thickness) grown on SRO(20 nm)/ STO(001) substrate with size dimensions of 5x5 mm were measured.

An example of such measures is shown in Figure 1, for a BFO film of 25 nm thick. The CTRs rods show the typical oscillations of a well ordered 2D-film. The figure shows some BFO corrected reflections by background, beam and experimental measuring geometry.

The measurements performed in the film with a thickness of 50 nm revealed an ordered bulk oxygen deficiency along the surface normal film direction. This new ordering shows a (2x2x2)-3Dimensional

periodicity as shown in Figure 2. Two data sets were consequently measured for this new structure: CTRs (Crystal Truncation Rods) corresponding to the interface between the substrate and the film and a set of FORs (fractional order rods) of this vacancy ordering structure (to determine its bulk periodicity) plus a set of rocking scans of each of the bulk Bragg reflections belonging to the film vacancy structure.

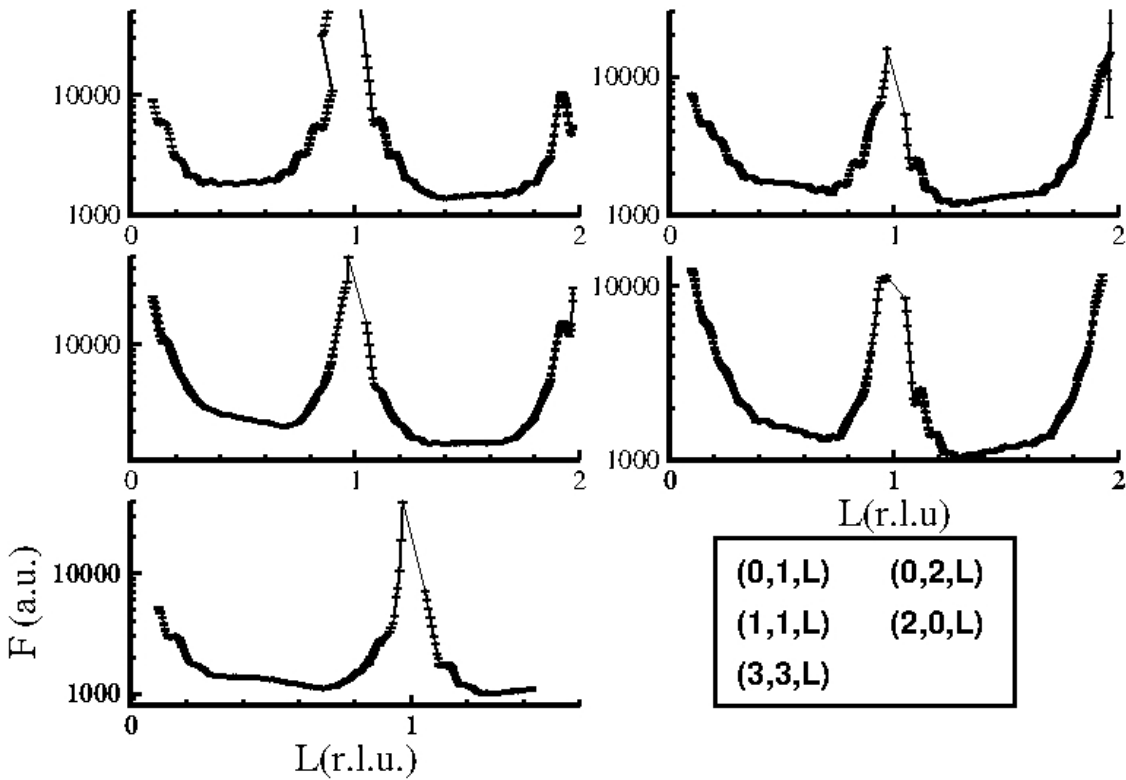


Figure 1. Corrected CTRs of the film  $\text{BiFeO}_3/\text{SrTiO}_3(001)$  with a thickness of 25 nm. The periodicity of the oscillations does not correspond solely to the thickness of the BFO film due to the possible contribution of the 10-15 nm thick SRO buffer layer that grows epitaxially with the substrate.

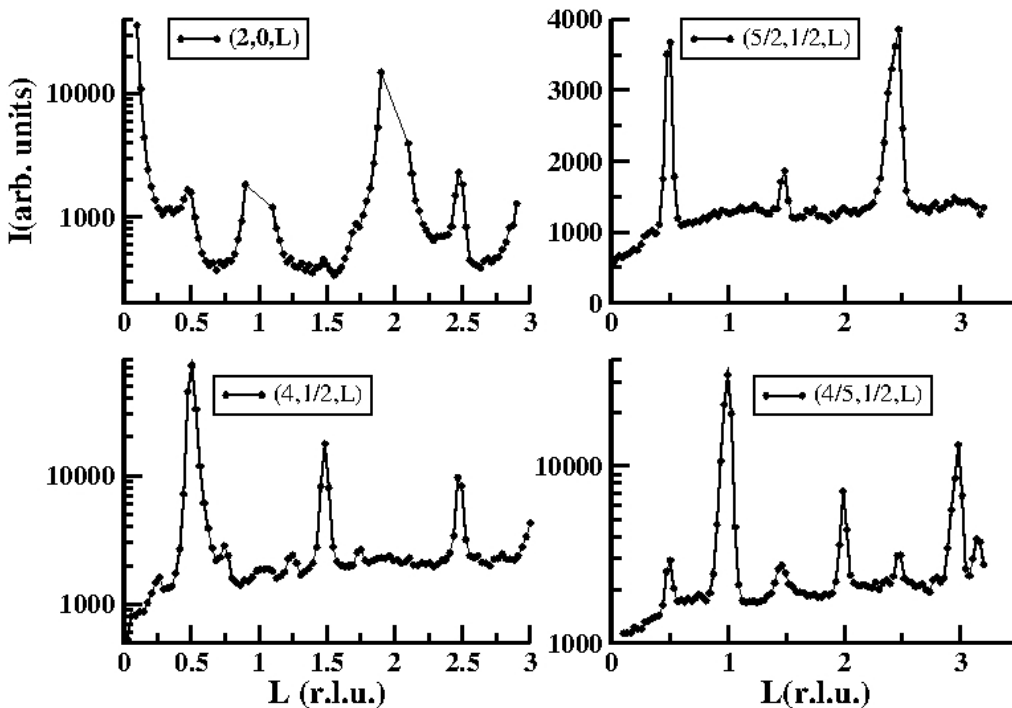


Figure 2. Figure 2. CTR and d FOR of a 50 nm thick BFO film. Peaks located at fractional integer  $L$  values denote the double periodicity of the structure along the 3 spatial directions  $(x,y,z)$ .

Due to the large data sets measured, the analysis of the data is still ongoing.