In-situ real time structural response of PMN-(0.32)PT

Experimental Report BM 28 01 892

A single crystal of Pb[$Mn_{1/3}Nb_{2/3}$]O₃-0.32PbTiO₃ (PMN-PT) was mounted on an insulating substrate of sapphire and mounted on Al2O3. The electrical contacts were placed on the electroded (110) faces, the beam penetrated the (100) face. The crystal was poled long the <100> direction.



The set up of the crystal in relation to the X-ray beam. The (100) face is perpendicular to the page.

An oscillating electric field was applied to the crystal and the response of the diffraction pattern was measured. Four frequencies were used for the application of the electric field; 0.01, 0.1, 1 and 10Hz

for the 200 peak, three frequencies for the 220 and 222 peaks, 0.01, 0.1, and 1Hz. At 0.01Hz the diffraction data were collected over one cycle, at 0.1Hz the diffraction data were averaged over four cycles and at 1Hz 20 cycles were averaged and at 10Hz 200 cycles were averaged.

The data is shown in its raw form below. The variation of counts at a point in reciprocal space is shown in green whilst the electric field is shown in blue demonstrating the phasing of the electric field and diffraction measurement is working.



Figure Raw data for the 2 0 0 reflection shows the applied voltage (blue) and diffraction counts (green).

Analysis of the peaks was carried out with Rietveld refinement in order to obtain a phase percentage of each of the two structures These present. were P4mm for the tetragonal phase and Cm for the monoclinic phase. The phase percentage is related to the peak It enables shape.

the phase fraction to be determined as a function of applied voltage. This is shown in the diagrams below



Figure shows the Rietveld refinement of the 2 0 0 peak, Cm phase (left) and Pmm phase (right).

In order to determine the peak extent as a function of applied voltage a number of mesh plots were taken, these are shown below for the

2 0 0 and 2 2 0 peaks. The complex microstructure arising from evolving domains can clearly be seen in the long tail perpendicular to the theta-two theta direction.



Showing the 2 0 0 peak (left, 2 2 0 peak centre and the displacement of the 2 0 0 peak at 0 and 4 kV mm⁻¹

The diagram below shows how the refined phase percentages vary as a function of applied electric field. We are analyzing the data which, so far, substantiates our hypothesis that the phase transition is frequency dependent and that there is a spontaneous polarization driving the Cm phase to the Pmm phase and vice vera.



Shows the tetragonal phase percentage with applied voltage.

This was the first part of our strategy to create a world-leading system for situ, real time measurements of electric displacement in response to an applied magnetic field, or magnetic polarisation in response to an applied electric field, whilst simultaneously mapping the accompanying crystal strain and structural distortions. In

this way, we aim to elucidate the origins of the microscopic coupling mechanisms present in these materials.