

**Experiment title:**Anomalous negative pyroelectric response in PbZrO₃-based perovskites**Experiment number:**

08-01-1077

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Report:

Absorption data has been acquired for the samples PZT1 and PZT2 at different temperatures. Both PZT1 and PZT2 are compounds of Pb(Zr,Sn,Nb,Ti)O₃ composition and perovskite crystal structure, but with different Sn/Zr stoichiometric ratio. At least two spectra have been acquired for each temperature, but where possible even more, in order to ensure the possibility to properly assign uncertainties to quantities extracted from EXAFS fitting procedures.

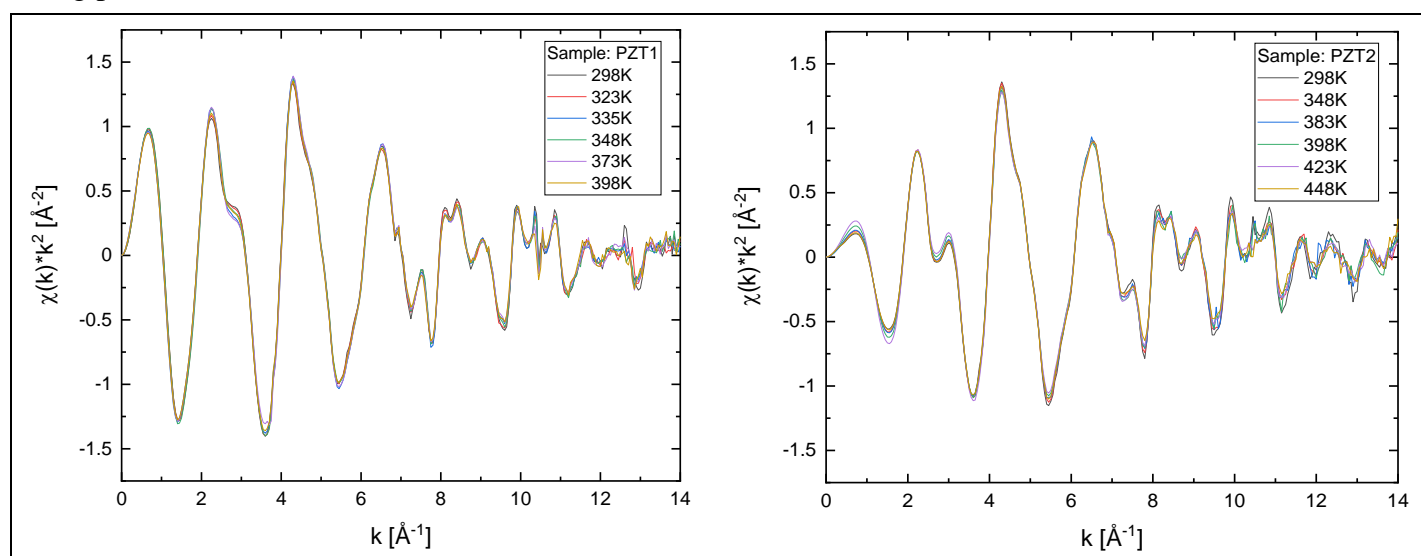


Figure 1: Zr K-edge EXAFS signals collected in samples PZT1 (left) and PZT2 (right) at different temperatures.

The acquisition of the absorption spectra generally seems to be repeatable, i.e. the spectra at each temperature show little dispersion, although some glitches are present in the high energy region. Figure 1 shows the Zr K-edge EXAFS signals measured for both PZT1 and PZT2 samples as a function of temperature.

In order to better appreciate the temperature trend of the data, in Figure 2 the Fourier Transform of the EXAFS signals have been reported. A prominent peak structure between 1 and 2 Å, related to backscattering from nearest neighbouring oxygen atoms, is clearly observed; several other peaks are visible at higher R values, involving the scattering from other metal/oxygen atoms, with some features common to both samples.

The analysis is still ongoing, but it is reasonable to think that the acquired data are sufficient to extract information on the local structural distortion in PZT1 and PZT2 sample in order to shed light on the enigmatic ferroelectric transition of such PbZrO_3 -based materials.

During the experiment, we had time to collect further EXAFS spectra in other similar PbZrO_3 -based samples.

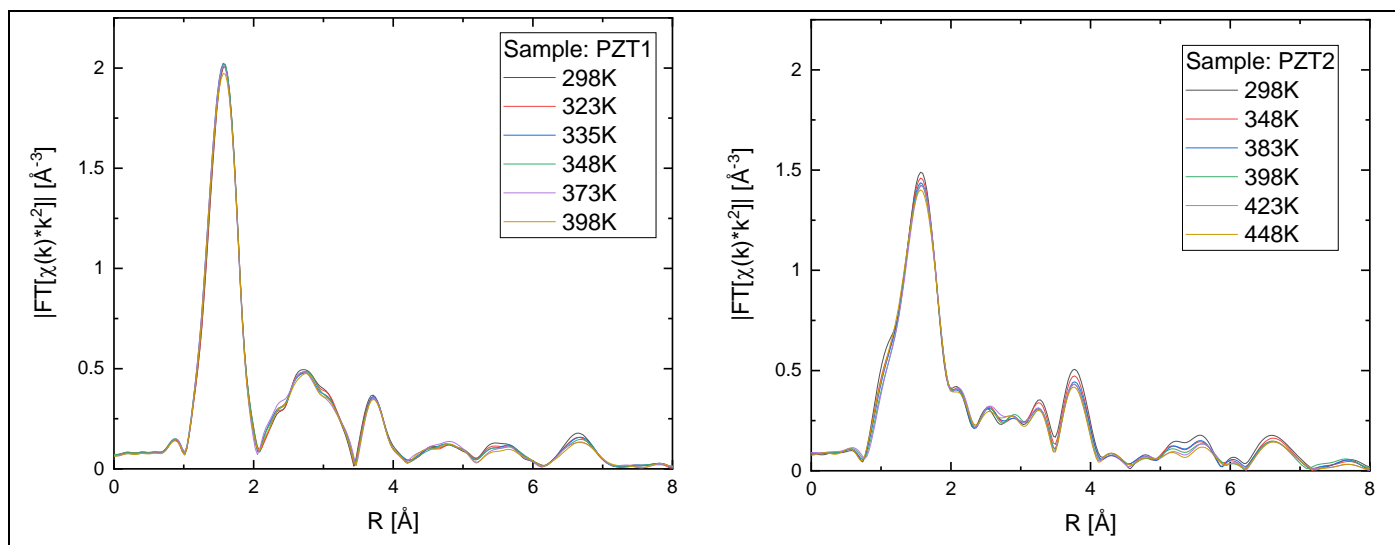


Figure 2: Fourier Transform of k^2 -weighted EXAFS signals for the sample PZT1 (left) and the sample PZT2 (right) at different temperatures.