Experimental report for Exp 02-02-841

We have successfully carried out a series of diffraction experiment on a PSN single crystal.
We observed R- and M-type SSR.

These SSR persist down to 20K and their intensity evolution are consistent with a simple decrease of thermal agitation and expected evolution of the lattice. No additional phase transition was detected down to the lowest temperature.

There are three main origins for additional periodicities in perovskite ferroelectrics : chemical order, rotations of oxygen octahedra, and cation displacement.

The existence of R-type SSR of the (h/2 h/2 h/2)-type are consistent with the partial chemical order observed on other PSN compounds. This chemical ordering of Sc and Nb atoms along the [111] direction is consistent with these SSR. The contribution of oxygen octahedra rotations to such SSR is forbidden by symmetry. We therefore tentatively attribute these SSR to the chemical order. Under this hypothesis, the ordering factor is of 100%. This order will be confirmed by HR TEM and measurements above the transition temperature. Indeed, in the paraelectric phase, there will not be any contribution from cation displacement as the unit cell is Fm-3m.

The M-SSR cannot be all attributed to in-phase rotations of oxygen octahedra. Indeed, SSR of the <h/2, h/2, l> type are observed despite being forbidden by symmetry for corner-sharing BO6 rotations. Such SSR have been attributed to anti-parallel displacement of cations, and the corresponding materials have been said to be antiferroelectrics.

The temperature evolution of these SSR does not indicate any drastic change from room temperature to low temperature.

A structural refinement from our data is under way to determine which type of cation displacement is at the origin of these SSR and prove or disprove the antiferroelectric nature of this sample. We shall corroborate this nature through ferroelectric measurements.

Resonant X-ray scattering data were acquired at various temperatures in order to determine the local structure around Pb and Nb ions. The analysis is under way by Stephane Grenier.

The perspectives offered from this novel understanding of the structure are :
- from structure refinement determine a structural model for these SSR that would shed light on the type of displacement leading to these SSR
- from resonant X-ray data to understand the local structure of the Pb and Nb ions in order to corroborate the global structure and gain a better understanding of the local environment, the effect of chemical order on the displacement of the Nb and the behavior of lead and its lone-pair in such a system.