**Experimental report for beamtime HC3408 : Lattice dynamics and phonon anomalies of Bi2SiO5**

This report presents a survey of the lattice dynamics of Bi2SiO5 (BSO), which was recently shown to be ferroelectric at room temperature [1]. This compound presents a great deal of technological interest because, unlike perovskite materials where the ferroelectricity arises from the cation off-centering, the ferroelectricity in BSO arises from the tilt of the quasi-1D tetrahedral silicate chains. The new possibilities for engineering tetrahedra-based ferroelectrics in contrast to octahedra-based materials thus urges for a deeper understanding of the physical properties underlying the occurrence of ferroelectricity in quasi-1D BSO. For this reason we report here an extended overview in reciprocal space of the lattice dynamics of BSO accross the ferroelectric transition using synchrotron techniques : Thermal Diffuse Scattering (TDS) and Inelastic X-ray Scattering (IXS), combined with DFT calculations.

While it is known from previous Raman data that the paraelectric – ferroelectric transition (TC = 663 K) is driven by the freezing of the polar soft mode at the Gamma-point [1], our data clearly evidence an additional phonon anomaly at the Brillouin zone boundary, giving rise to characteristic TDS features. Using energy and momentum resolved measurements, we observed the substantial but finite softening of the Y-point transverse optic (TO) phonon branch, which is accompanied by a suppression of the transverse acoustic (TA) frequency induced by TO-TA mode repulsion, indicating a strong TO-TA mode coupling. Our experimental results are validated by our DFT calculations, and provide direct evidence for a strong competition between ferroelectric and anti-ferroelectric ordering, thus opening the route towards the exploration of the boundary between these two phases in BSO and other similar systems.

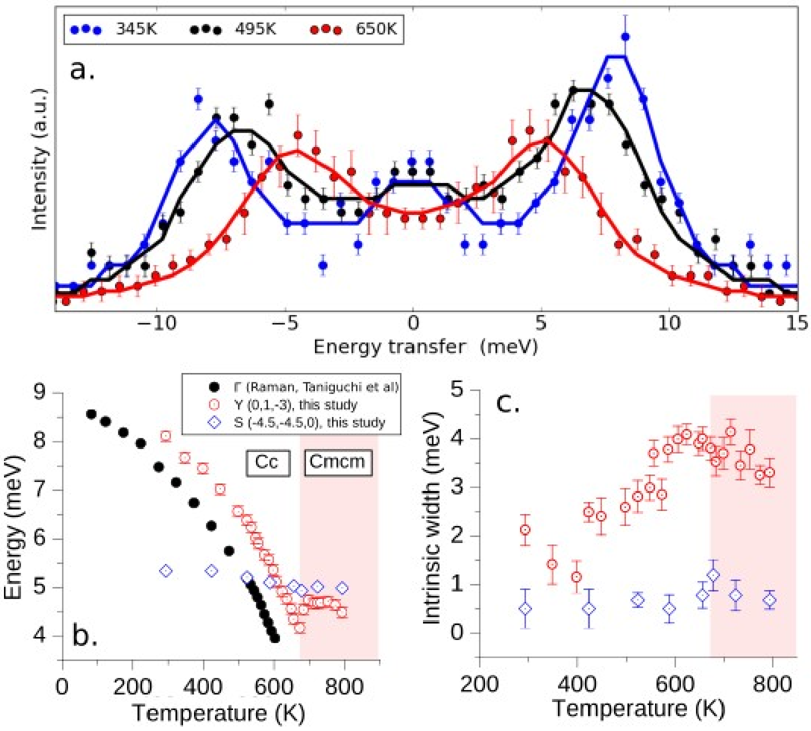


Figure 1 : a. IXS spectra measured at the Y point for three different temperature: 345 K (blue, T << $T_C$ ), 495 K (black, T < $T_C$ ) and 650 K (red, T~$T_C$ ). b. Temperature evolution of the phonon energies at the Y point (red), S point (blue) and Γ point (black). The Γ point data correspond to the FE soft mode and correspond to the Raman data. c. Evolution with temperature of the intrinsic width of the phonon excitations at the Y and S points.