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Archetypal Soft-Mode Driven Antipolar Phase Transition in Francisite Cu3Bi(SeO3)2O2Cl

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Antiferroelectricity can be seen as being a property similar to antiferromagnetism with electric dipoles instead of spins. It is characterized by a phase transition between a high- and a low-symmetry phase where antiparallel dipoles emerge [1]. In analogy with soft-mode driven ferroelectric transitions (e.g. in PbTiO3), it is then possible to think of an ideal antiferroelectric phase transition driven by an "anti-polar soft-mode", which is a soft phonon mode related to antiparallel ionic displacements [2]. However, such a phase transition has not been observed yet; instead, classical antiferroelectric transitions are usually of the order-disorder type.

In this study, we show that francisite (Cu3Bi(SeO3)2O2Cl) undergoes such an anti-polar soft-mode driven phase transition. Francisite is an orthorhombic crystal that has a phase transition from space group Pmmn to Pcmn at 115 K [3]. This phase transition induces a doubling of the unit cell along the c axis, which folds the zone-boundary Z point (0,0,1/2) of the high-symmetry phase onto the Γ point in the antipolar phase [4]. We measured the low-frequency phonon modes in both phases using a combination of Raman spectroscopy, Inelastic X-Ray Scattering (IXS) and Thermal Diffuse Scattering (TDS). IXS and TDS measurements have been performed at the ID 28 beamline of ESRF [5].

Raman spectra across the phase transition are shown on Fig. 1. and show a clear soft phonon mode visible only in the low-temperature phase. The soft-mode above Tc on the other hand is seen in the IXS spectra and in the TDS intensity. Fig. 2 shows the combination of experimental data with the soft-mode energy squared as a function of temperature. It displays a typical soft-mode behaviour in the vicinity of Tc, with deviations originating from mode coupling with other low lying phonon modes. The slopes of E2 vs. T indicate that the transition is close to tricritical.

Fig. 1 is the enclosed "Raman_cascade.jpg" file and Fig 2. is "Soft-mode_evolution.jpg"

Summary

Topic

1. Multiferroics and ferroelectrics

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