



	Experiment title: Intrinsic orthorhombic distortion in Sr_2IrO_4	Experiment number: HC5260
Beamline: ID28	Date of experiment: from: 21/02/2023 to: 23/02/2023	Date of report: 11/09/2023
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Report:

The main goal of our experiment was to look for intrinsic orthorhombic distortions in nominally tetragonal Sr_2IrO_4 . Such deformations are expected to appear as a splitting of Bragg peaks. Fig. 1 shows the reciprocal space maps in the HK0 and H0L planes obtained for our single crystal Sr_2IrO_4 , at a temperature well below the antiferromagnetic Neel temperature $T_N \sim 240$ K, below which the intrinsic orthorhombicity is expected to appear. Unfortunately, such Bragg peak splitting is not observed. We also performed the experiment in the high resolution configuration. These data could not be refined properly due to multiple scattering arising from loosely coupled crystal flakes along the c-axis (visible as streaks along [001] axis in Fig. 1). However, directly inspecting the detector images also revealed no splitting implying that the orthorhombic distortions, if any, are below the resolution limit of the instrument. We spent a total of 1 day on the measurements of Sr_2IrO_4 .

With the additional day available, we looked at a back up sample of single crystal Ca_2RuO_4 . This choice was motivated by the highly anomalous structural properties exhibited by the system [1]. Fig. 2 displays reciprocal space maps taken at 80 K and 360 K for HK0 plane, and at 360 K for H0L and 0KL planes. Clear thermal diffuse scattering features are observed in the data which implies soft phonon modes in extended regions of the Brillouin zone, which has never been reported previously. Future non-resonant inelastic x-ray scattering measurements will focus on measuring phonons in this material.

In conclusion, the experiment was very successful. Although the orthorhombic deformation in Sr_2IrO_4 could not be detected, the results on Ca_2RuO_4 are extremely promising and have motivated us to carry out further investigations in this material.

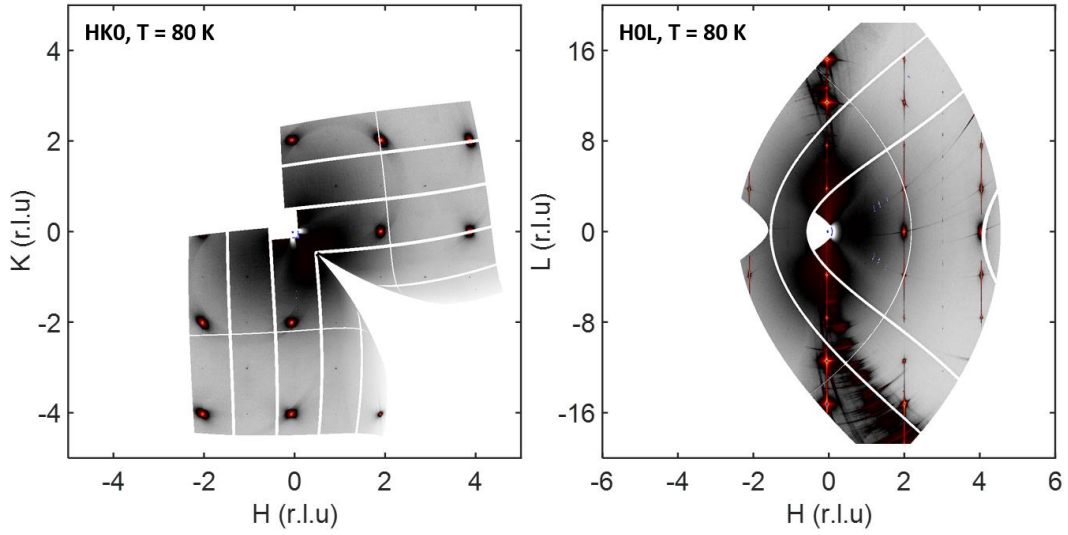


Fig. 1: Diffuse x-ray data obtained for Sr_2IrO_4 at $T = 80$ K in the HK0 and H0L planes.

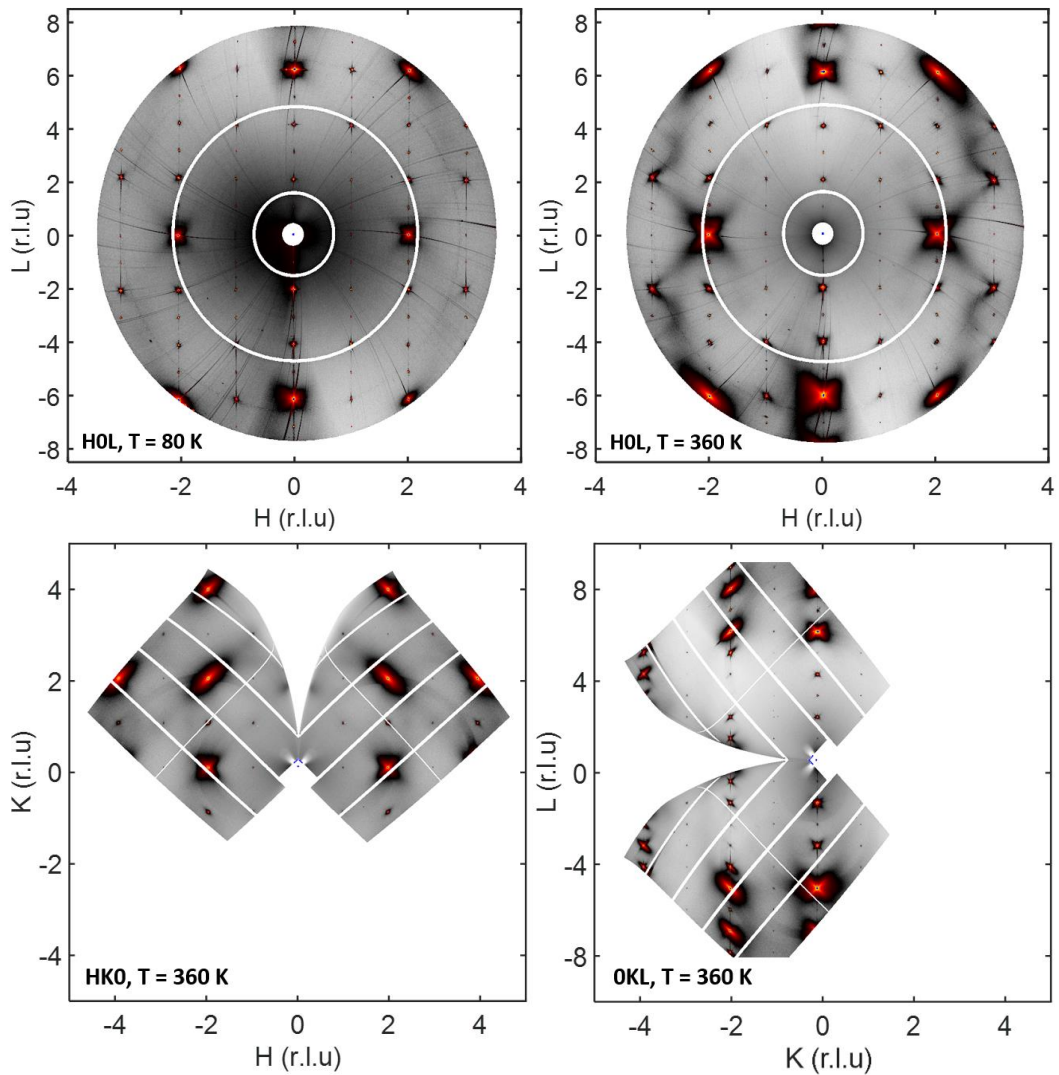


Fig. 2: Diffuse x-ray data obtained for Ca_2RuO_4 at $T = 80$ K and $T = 360$ K in the H0L plane and $T = 360$ K in the HK0 and OKL planes. Clear thermal diffuse scattering features are observed in the H0L plane in extended regions of the Brillouin zone, implying strong phonon softening.