Resonant X-ray Scattering of $Co_3Sn_2S_2$ Reveals Unexpected Charge-Order Peak

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Introduction

What is $Co_3Sn_2S_2$?

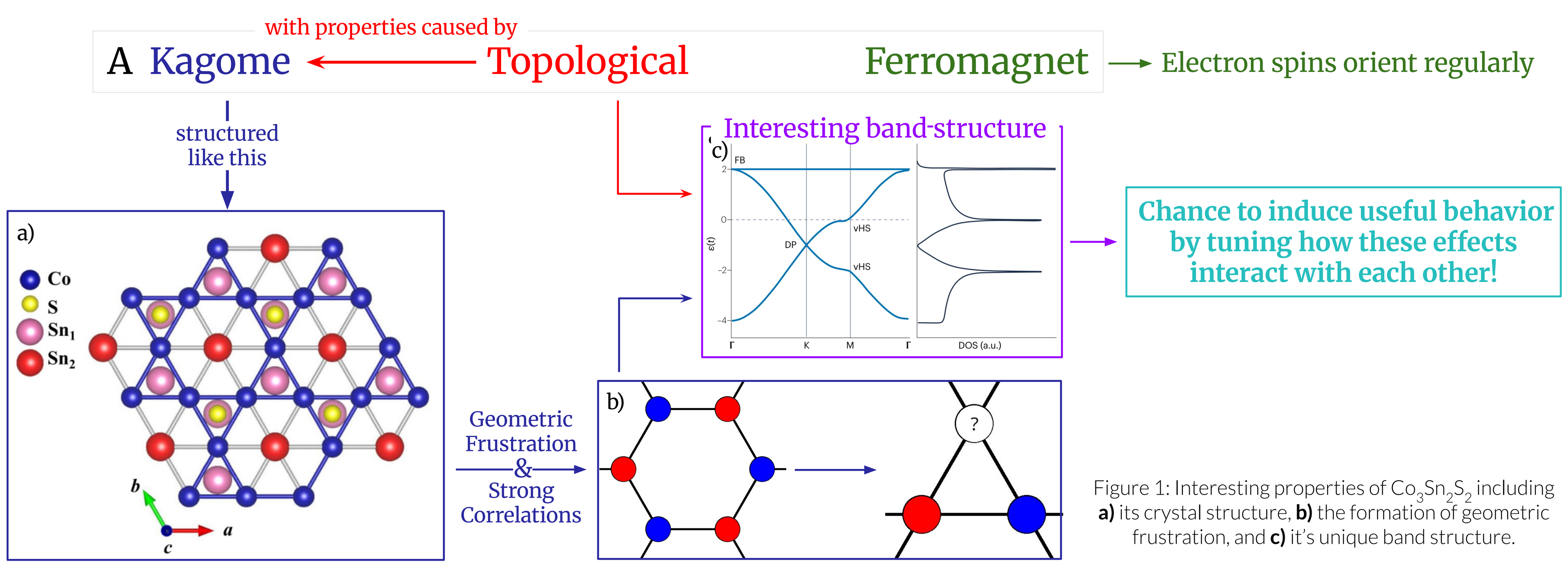

Figure 1: Interesting properties of $Co_3Sn_2S_2$ including **a)** its crystal structure, **b)** the formation of geometric frustration, and **c)** it's unique band structure.

Why is this interesting?

Kagome materials exhibit many interesting properties including topological order, strong electron correlations, and the formation of a large anomalous quantum hall effect. Many of these arise from the unique band structures that result from the geometric frustration imposed by the lattice. Their complex interplay can then form uncommon phases such as unconventional superconductivity.[1,2]

Along with offering-up the opportunity to investigate these unique behaviors, these coexisting orders can be tuned via doping or strain.[1] This makes kagome materials ideal candidates for novel quantum technologies such as efficient, fault-tolerant quantum computing!

Here, we use x-rays to probe the kagome sublattice formed by the cobalt atoms in $Co_3Sn_2S_2$ in order to gain insight into the relationship of the material's magnetic states with a charge-order peak.

Methods

Resonant X-ray Scattering

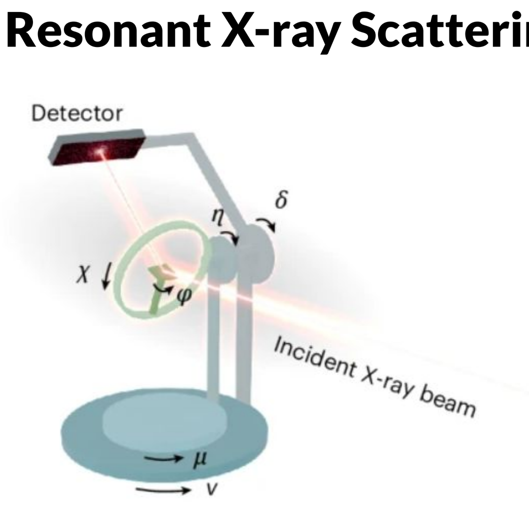

Figure 2: Diffractometer setup

Reciprocal Space

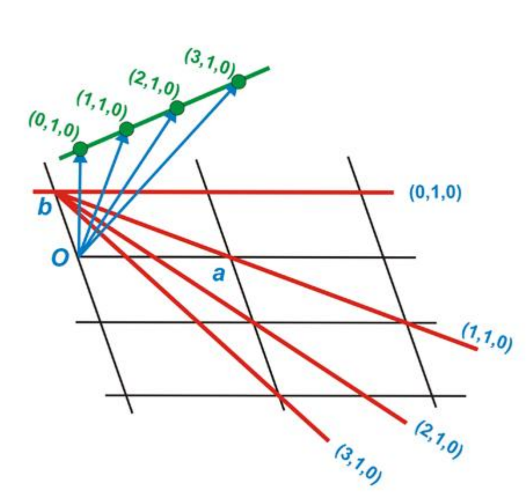

Figure 3: Mapping from real to reciprocal lattice space

Unexplained Peak in LCLS experiments

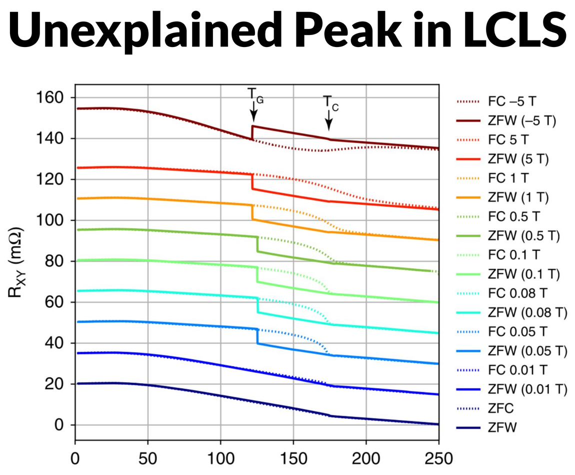

Figure 4: Resistance as a function of temperature in $Co_3Sn_2S_2$ upon heating (solid) and cooling (dotted)

Multiple magnetic phases have been proposed for $Co_3Sn_2S_2$, but there is disagreement on their exact description.[3–5] In order to collect more data on this ordering, XPP studies were conducted at LCLS to measure the time-evolution of this phase.

By probing the cobalt K-edge (inner electron shell) at ~7.7 keV, we are able to characterize periodic ordering of the electrons involved in the formation of the magnetic phases in $Co_3Sn_2S_2$. However, the LCLS study revealed a previously unreported charge-order peak which persists across a wide temperature range.

This is particularly interesting because electronic and magnetic orderings are predicted to not typically coexist in kagome materials. Electronic orderings (such as superconductivity) tend to arise when same-site interactions dominate, whereas magnetic orderings tend to correspond to when nearest-neighbor effects dominate.[1] The appearance of both in a single material suggests a coupling between electronic and magnetic orders. This offers a unique opportunity to study whether these orders enhance one another or compete.

Results

Preprocessing Improvements

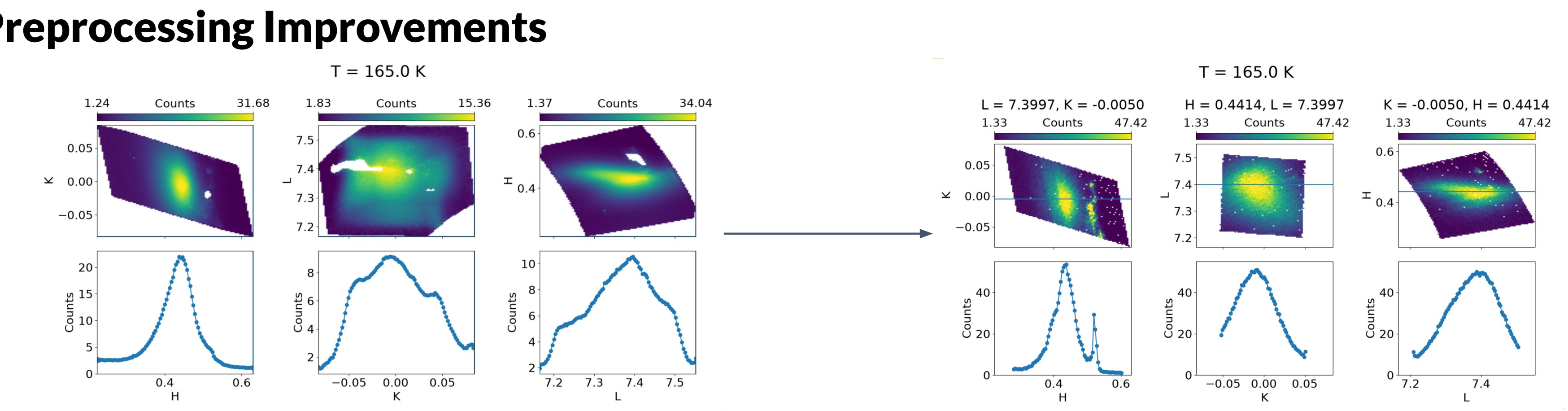

Figure 5: 2d and 1d representations of the measured intensity at 165K as generated by the original method of averaging over the entire dataset (left) and the new method of averaging over thin slices about the peak (right). The missing sections in the left image correspond to artifacts that were manually masked out.

In order to understand how this peak is structured, we would like to analyze its periodicity independently in the three lattice directions. Our initial analysis did this by averaging over the other two axes. This indicated a single peak in H, a 3-peak structure in K, and a complex, multipeak structure in L.

However, we realized that **by averaging over thinner slices, we see a better representation of the true structure!** This method reveals that the K and L data are both single-peaked, while the H data has a single peak and has 1-2 satellite peaks.

Fitting the New Data

We were then able to fit this data to a series of asymmetric Voigt functions. Fitting the K and L datasets is straightforward as they can be modeled as a single peak, however, the H data is multi-peaked, so the fitting process has to be more in-depth. To ensure that we accurately model the satellite peaks as corrections to the central effect, an iterative process was used. This involves making initial guesses for each peak and refining each one individually such that the corrections are preferentially applied to the satellite peaks. These individual fits then serve as initial guesses for a final fitting pass over the combined function to fine-tune the entire fit.

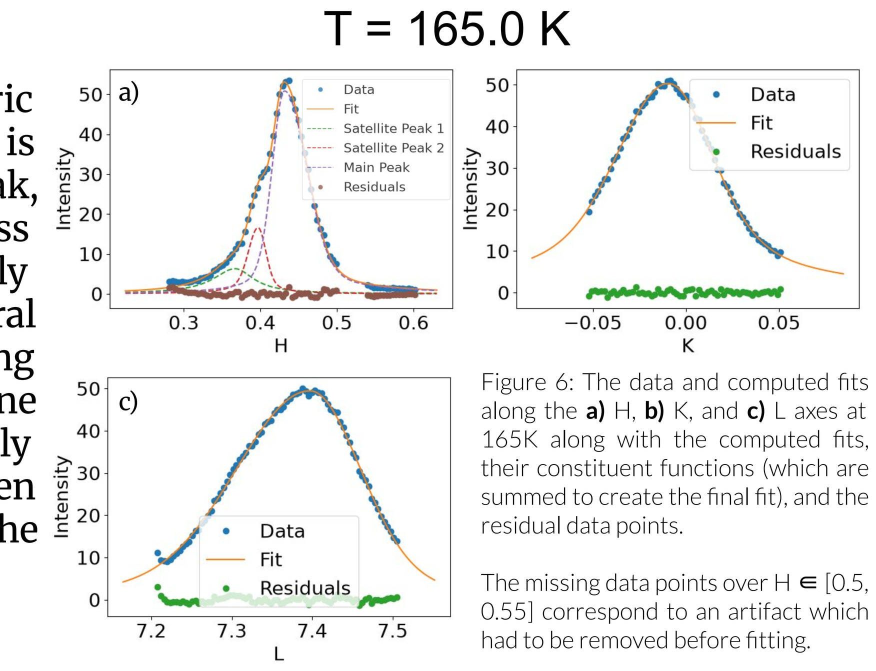

Figure 6: The data and computed fits along the **a)** H, **b)** K, and **c)** L axes at 165K along with the computed fits, their constituent functions (which are summed to create the final fit), and the residual data points.

The missing data points over H ∈ [0.5, 0.55] correspond to an artifact which had to be removed before fitting.

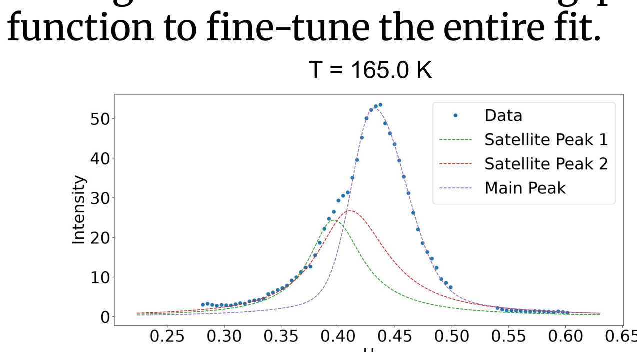

Figure 7: The initial guesses for each peak of the 165K H-fit

Analysis

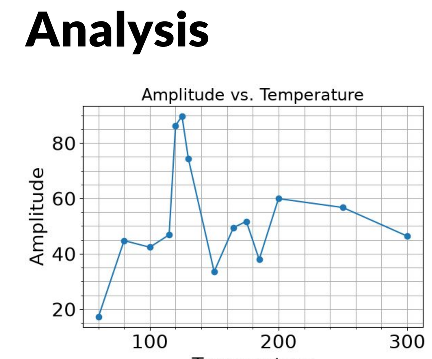

Figure 8: The amplitude of the peak as a function of temperature

We firstly note that this peak is maximized around 125K. (Fig. 8) This is the same point at which the magnetic transition is observed. This could be an indication that the magnetic disorder associated with this transition is responsible for driving the charge-order.

We can also note that because of the 125K maximum, the satellite peaks in H become less-significant near the transition temperature as their amplitude does not increase proportionally with that of the main peak. (Fig. 9) This suggests that they may originate from different charge-order phases.

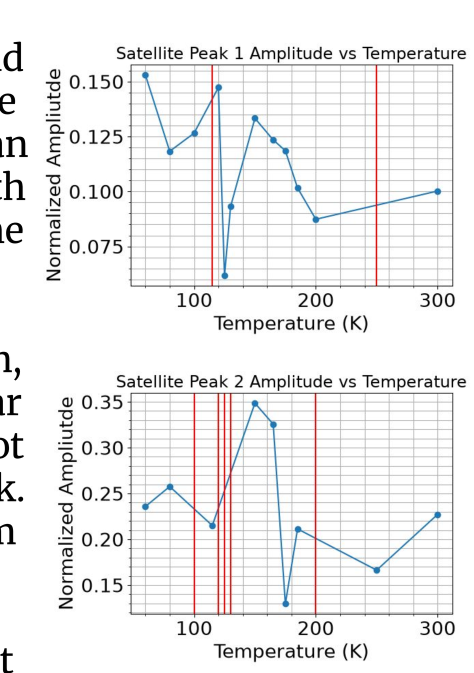

Figure 9: The amplitude of the H satellite peaks normalized against the amplitude of the main peak as a function of temperature.

The red lines indicate temperatures where no satellite peak was necessary to fit the data.

Lastly, investigating the ratio of the half-height half-widths of the L peak (Fig. 10) reveals that the peak becomes very asymmetric near both the 125K and 165K transitions, but in opposite directions, this could indicate that there is an unresolved satellite peak corresponding to additional charge-order modulation that is suppressed at the lower magnetic transition and enhanced at higher temperatures. This would be consistent with the two types of magnetic orders being distinct from each other.

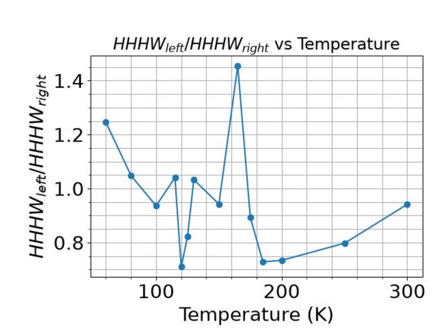

Figure 10: The ratio of the left to right half-height half-widths along the L axis as a function of temperature

Conclusion

Here, we have successfully performed an initial characterization of an unexpected charge-order peak in $Co_3Sn_2S_2$. We find behavior consistent with the existing reports of magnetic orderings and evidence that the two types of order are interacting. Moving forward, we would like to build on these results by running tests in a magnetic field in order to interrogate the interaction between the electronic and magnetic orderings. We would also like to test a finer and wider temperature sweep in order to refine the positions of the various transitions and conduct XPP/XPCS experiments at LCLS to learn about their time-evolution dynamics.

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IMAGE REFERENCES

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