Experimental report

21/12/2020

Proposal: **5-24-649** **Council:** 10/2019

Title: Lattice distortions in the pressure-induced plaquette phase in the Shastry-Sutherland compound, SrCu2(BO3)2

Research area: Physics

This proposal is a new proposal

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Samples: SrCu2(BO3)2

Instrument	Requested days	Allocated days	From	To
D20	6	4	29/01/2020	31/01/2020

Abstract:

We propose a powder diffraction experiment at D20 to determine the lattice symmetry of SrCu2(BO3)2 in the plaquette phase. The Shastry-Sutherland lattice consists of spin pairs embedded in a square lattice and with inter-dimer coupling, J, and intra-dimer coupling J'. It has an exact dimer product ground state for J'/J <= 0.675. Upon increasing the ratio of J'/J, the system goes through a quantum phase transition to a plaquette singlet state followed by a transition to a Néel phase. SrCu2(BO3)2 is unique since it is topologically equivalent to the Shastry-Sutherland lattice. The ratio, J'/J, may be tuned by applying pressure and the resulting phase diagram resembles that theoretically predicted for the Shastry-Sutherland model. The nature of the plaquette phase in SrCu2(BO3)2 is still debated and recent theoretical studies suggest that the magnetic order in this state may be accompanied by an orthorhombic lattice distortion. With the proposed experiment we aim to identify this distortion and thereby gain a better understanding of the plaquette phase.

Lattice distortions in the pressure-induced plaquette phase in the Shastry-Sutherland compound, $SrCu_2(BO_3)_2$

Proposal no: 5-24-649
Beamtime: D20, 2 days
Experiment team: Mohamed Zayed (Carnegie Mellon University Qatar), Gaétan Giriat and Ellen Fogh (École Polytechnique Fédérale de Lausanne)
Local contacts: Thomas Hansen, James Maurice

The Shastry-Sutherland (SS) lattice consists of spin pairs (dimers) embedded in a square lattice (see Fig. 1a) and with inter-dimer coupling, J, and intra-dimer coupling J'. It has an exact dimer product ground state for $J'/J \leq 0.675$ [1]. Upon increasing the ratio of J'/J, the system goes through a quantum phase transition to a plaquette singlet state followed by a transition to a Néel phase [2]. $SrCu_2(BO_3)_2$ (SCBO) is a unique material since it is topologically equivalent to the SS lattice [3]. With $J'/J \sim 0.6$ close to the critical point, SCBO presents remarkable experimental testing grounds for the SS model. The ratio J'/J may be tuned by applying pressure and the resulting phase diagram resembles that theoretically predicted for the SS model [4] (see Fig 1b).

In this proposal, we focus on the plaquette phase residing in the pressure region 1.8-4.0GPa. Here, existing experimental results are limited and appear to contradict theoretical predictions. Both an NMR study [5] and inelastic neutron scattering study [4] suggest the diamond (or full) plaquette as opposed to the predicted square (or empty) plaquette [6]. Another theoretical study even proposes that there might be two intermediate phases rather than a single one [7] and thus the magnetic structure in the plaquette phase remains debated.

The square plaquette preserves the C_4 symmetry of the SCBO tetragonal lattice and all Cu sites remain equivalent. On the other hand, the C_4 symmetry is lost in the diamond plaquette phase and now two different Cu sites exist. Likewise, reflection symmetries, σ_{xy} and $\sigma_{x\bar{y}}$, are broken in the square plaquette state but not in the diamond one. The orthorhombic distortion in the diamond plaquette phase is suggested to stabilize magnetic state [8,9] in analogy to the antiferromagnetic spin-1 chain, the so-called Haldane chain. Here, spin pairs group together such that the distance between neighbors to either side along the chain is no longer equal [10]. The magnetic state may thus induce a lattice distortion and this distortion is measurable using neutron diffraction.

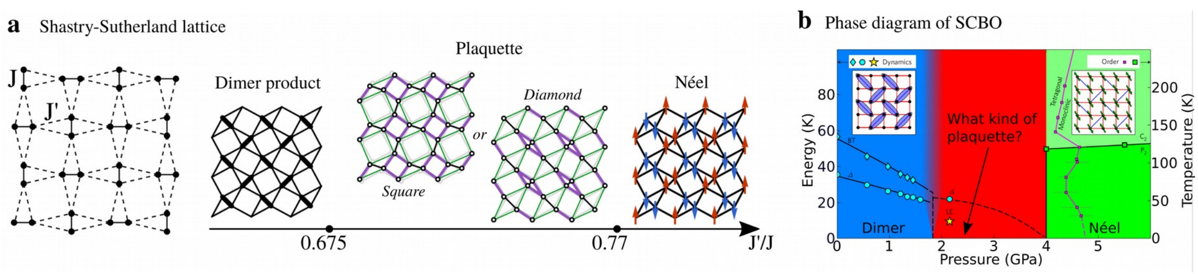

Figure 1: *(a) Illustration of the SS lattice with inter-dimer and intra-dimer coupling, J and J', respectively, as well as the theoretically predicted phase diagram. The nature of the plaquette state remains debated and is the very topic of this proposal. (b) Experimental phase diagram of SCBO under pressure.*

In order to address this question, we intended to perform a neutron powder diffraction experiment at D20 using a McWhan cell at pressures 2.0GPa and 2.5GPa and at temperatures below 2K. We used powder obtained from crushed SCBO single crystals to obtain the highest sample purity. However, the pressure cell was not cooperating and we only achieved a pressure of around 1.0GPa. More, the cryostat was also not operational for most of the time so in the end we could not reached the conditions we needed for this experiment. Figure 2 shows an overview of the data we collected. All data was taken at room temperature.

We have been allocated another 2 days but due to the covid pandemic, they have not been scheduled yet. Hopefully we can get to do this super exciting experiment in the beginning of 2021.

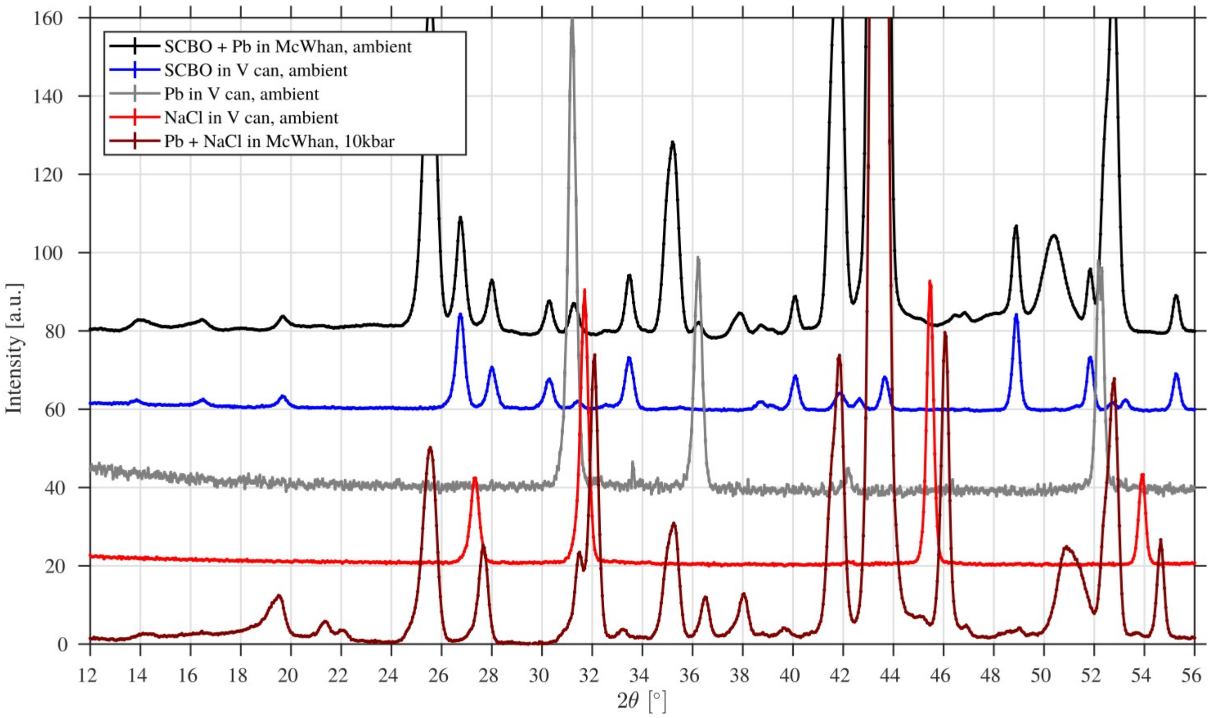

Figure 2: *Comparison of data for SCBO, Pb and NaCl in a vanadium can or in the McWhan with and without pressure.*

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