

**Experiment title:**High-pressure X-ray investigation of phase transitions in model quantum spin system  $\text{SrCu}_2(\text{BO}_3)_2$ **Experiment number:**  
HS-3692**Beamline:**  
ID9A**Date of experiment:**

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**Report:**

We performed synchrotron X-ray single crystal and powder diffraction measurements as a function of pressure and temperature in order to determine the structural phase diagram of the Shastry-Sutherland quantum magnet  $\text{SrCu}_2(\text{BO}_3)_2$ .

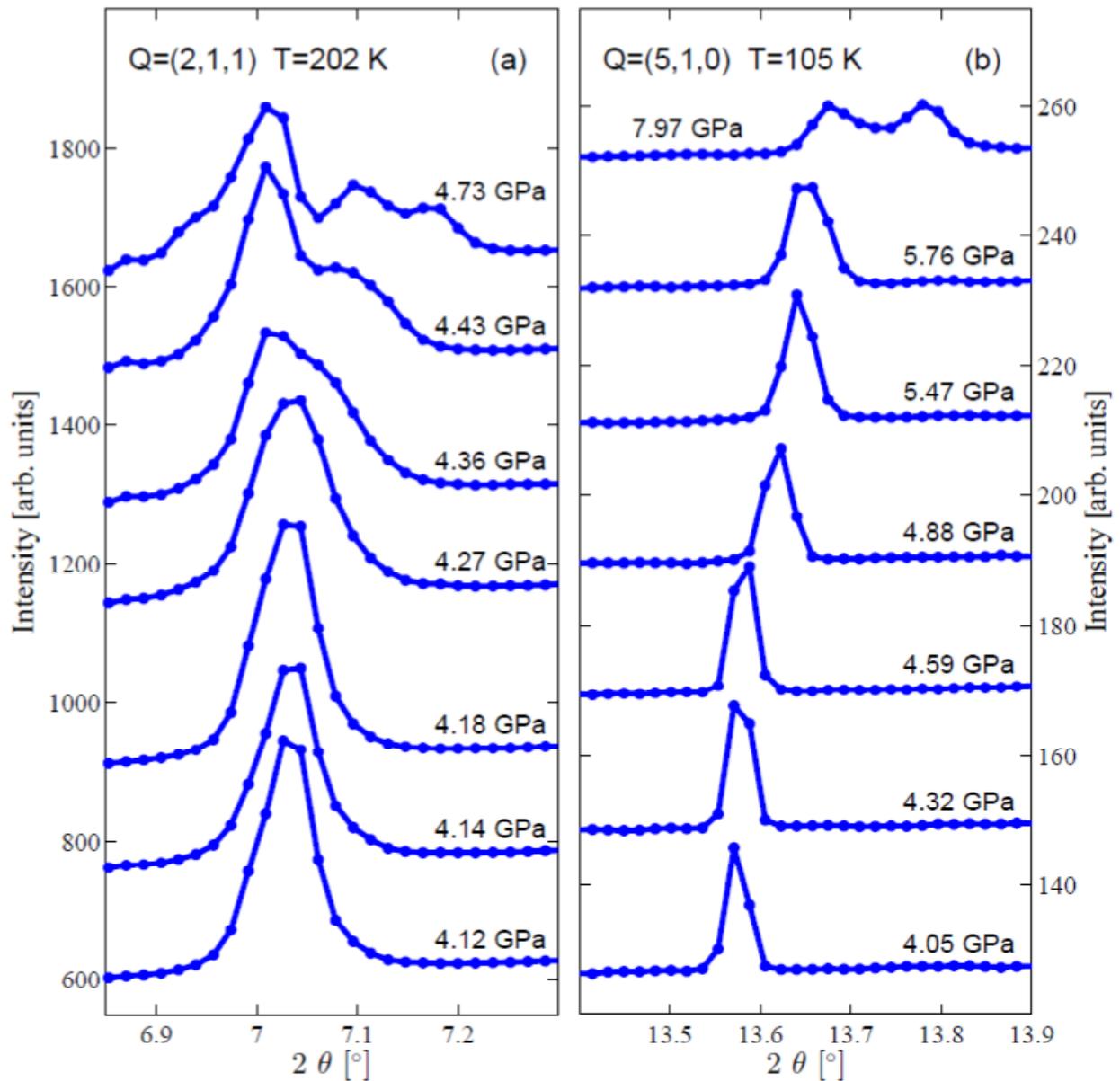
Hydrostatic pressure ranging from ambient to 19 GPa was applied to the samples by mean of a diamond anvil cell (DAC), with helium as pressure transmitting medium. Pressure calibration was performed using the ruby luminescence method. Temperature was varied from ambient to 25 K using a helium cooled cryostat.

The single crystal samples ( $\sim 30 \times 30 \times 5 \mu\text{m}^3$ ) were placed in the DAC with c-axis parallel to the X-ray beam and rotated by  $\pm 10^\circ$  during exposure while the powder samples were rotated by  $\pm 3^\circ$ .

We could observe the distortion from the ambient tetragonal to the monoclinic phase [1] and follow this transition as a function of temperature down to 30 K. The transition essentially remained confined in the 4 – 5 GPa range [2]. A higher pressure first order transition around 15 GPa was also observed.

A full refinement of the powder diffraction data was not possible due to the presence of impurities in the sample.

Figure 1 shows a typical peak splitting observed on ID9A with  $\text{SrCu}_2(\text{BO}_3)_2$  in the DAC for both a powder and a single crystal sample.



**Figure 1:** Pressure dependence of Bragg reflections in  $\text{SrCu}_2(\text{BO}_3)_2$ . (a) Powder sample,  $T=202$  K. The  $(2,1,1)$  tetragonal reflection splits into several non equivalent monoclinic reflections. (b) Single crystal. The original  $(5,1,0)$  tetragonal reflection abruptly changes position above 4.59 GPa. Above this pressure, the reflection broadens and can be fully resolved as two non-equivalent peaks around 8 GPa. Peaks are shifted vertically for clarity.

## References:

- [1] I. Loa, F.X.Zhang, K.Syassen, P.Lemmens, W.Crichton, H.Kageyama, Y.Ueda, *Physica B* 359–361, 980 (2005).
- [2] M. E. Zayed, Ch. Rüegg, E. Pomjakushina, M. Stingaciu, K. Conder, M. Hanfland, M. Merlini, and H. M. Rønnow, *Solid State Commun.* 186, 13 (2014).