



Experiment title: Pressure-induced spin state transition in CoCr_2Se_4 single crystals		Experiment number: 01-02-1002
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Report:

Experiment

Single crystals of CoCr_2Se_4 were studied as a function of pressure from 0.1 to 21 GPa at the SNBL BM01A at ESRF using PILATUS 2M detector with a 0.6997 \AA wavelength. Anomaly around 16 GPa, consistent with a spin state transition in the Co sublattice, was confirmed.

Results and discussion

At room temperature CoCr_2Se_4 adopts the monoclinic Cr_3S_4 -type structure and undergoes a first-order order-disorder transition at 750°C to the filled CdI_2 -type structure [1]. On cooling the monoclinic CoCr_2Se_4 phase undergoes an antiferromagnetic transition at $T_N = 230 \text{ K}$ as confirmed by our neutron diffraction experiments [2]. Together with magnetic, the electrical properties also change their behavior at 230 K [2].

Simultaneous changes in magnetic and electrical properties in CoCr_2Se_4 at 230 K can originate from the undergoing structural changes. From the previous pressure-dependent scans performed on the powdered CoCr_2Se_4 sample we have observed an anomaly consistent with a Co high- to low-spin state transition (Fig. 1, filled circles). The single crystal experiment on CoCr_2Se_4 confirmed the anomaly.

However, a small unit cell volume (260 \AA^3) and the limited opening angle of high pressure cells resulted in a low number of experimental reflections and induced correlation effects. Unfortunately, this hindered to obtain quality structural refinements for the experimental pressure points. Behavior of the unit cell volume with pressure for the obtained single crystal data is shown on the Figure 1, filled squares.

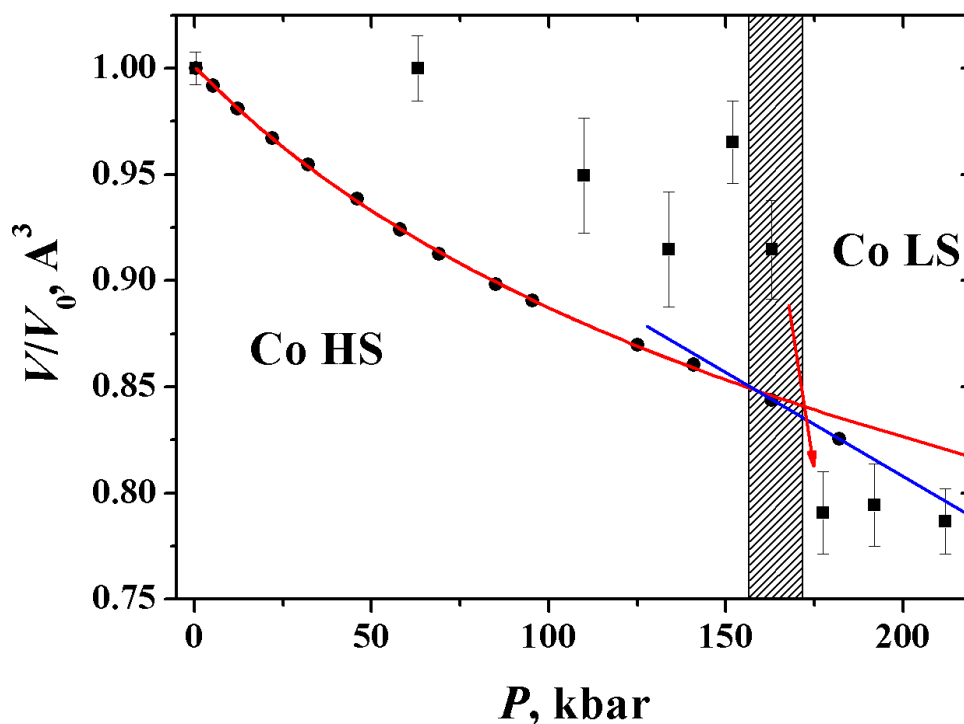


Fig. 1. Anomaly in the unit cell volume for CoCr_2Se_4 around 16 GPa. Filled circles correspond to the powder data, filled squares correspond to the single crystal data.

Summary

Anomaly around 16 GPa in the pressure dependent data for the CoCr_2Se_4 single crystals consistent with a Co high- to low-spin state transition was confirmed. Due to the induced correlations no reliable structural refinement was possible. To improve the data, an experiment with a shorter wavelength, i.e. 0.3 Å, could be required to cover more volume of the reciprocal space and to obtain datasets with a sufficient number of reflections.

References

1. Svitlyk V., Mozharivskyj Y. *Inorg. Chem.* **48**, 2009, 5296-302.
2. Svitlyk V., Mozharivskyj Y et. al. Unpublished data.