Experimental report

06/09/2022

Proposal: **5-54-346** **Council:** 4/2020

Title: Effect of uniaxial pressure on magnetic order and spin excitations ofNaFeAs

Research area: Physics

This proposal is a new proposal

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Samples: CsV3Sb5

Instrument	Requested days	Allocated days	From	To
IN22 CPA	6	6	28/09/2021	04/10/2021

Abstract:

An in-plane external uniaxial pressure has been effectively used as a method to acquire single domain iron pnictides, such as BaFe2As2 and NaFeAs, which both exhibit twin-domains without uniaxial strain below their respective tetragonal-to-orthorhombic structural (nematic) transition temperatures Ts. We have recently observed that such a strain on BaFe2As2 also induces a static or quasi-static out-of-plane (c-axis) AF order and its associated critical spin fluctuations near TN /Ts. Given this, and that previous work has shown that spin fluctuations respond to Ts in NaFeAs, we plan to use polarized elastic neutron scattering to study low-energy spin fluctuations in detwinned NaFeAs, which undergoes a magnetic and structural phase transitions at 45K and 58K respectively. In the case of BaFe2As2, these transition temperatures coincide, so we put forward the experiment detailed in our proposal to determine if uniaxial pressure can modify the magnetic structure of NaFeAs, and whether there is also spin fluctuation anisotropy induced by uniaxial pressure similar to the case of BaFe2As2.

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Sample change request: The sample and topic of the experiment has been changed has been changed. as the sample is incredibly air sensitive and would require careful preparation to survive the trip to France from Rice University. In the context of Covid19, we have decided not do that as the chance to prepare the sample properly was too risky. Further, the student in charge of the uniaxial device was not sure to be able to come to France as well. A change of sample request was accepted by the ILL direction in September 2021.

New title: "Loop currents in the Kagome superconductor CsV_3Sb_5"

Proposal: A chiral flux phase has been theoretically predicted in the topological superconductor AV_3Sb_5 (A = K,Rb,Cs) with quasi-2D Kagome lattice [Feng21]. These materials exhibit topological charge density wave as observed experimentally using X-ray that quadruples (2x2) the hexagonal structure [li21]. The proposed chiral flux state breaks time-reversal symmetry and displays anomalous Hall effect as it was long-sought-after by Haldane. Two very recent muons spin spectroscopy studies report time-reversal symmetry breaking below the charge order temperature (around 80 K) [Mielke22,Yu21], actually interpreted by loop current states which reminds those discussed in cuprates on which we have been working for years [Bourges21]. For instance, Mielke et al [Mielke22] propose a current pattern among the triangles of vanadium atoms but the exact LC pattern can only be deduced from diffraction techniques. Therefore, we propose to study these materials with polarized neutron diffraction on IN22. They represent new platforms to investigate the interplay between topology, unconventional superconductivity and strong electron–electron correlations. The experiment is straightforward as the expected magnetism would occur at momentum positions where the nuclear scattering is absent or weak. Neutron polarization is necessary to remove the non-spin-flip background as the expected signal should be weak. This material is a nice opportunity to show that loop currents can exist in a wider range of quantum materials.

Experimental team: P. Bourges, D. Bounoua, Y. Sidis, F. Bourdarot, M. Klemm, Pengcheng Dai

Report:

Figure 1 shows the hexagonal structure of CsV_3Sb_5 and the Kagome lattice of vanadium atoms. Figure 2 shows possible loop currents structure on the David star of the Kagome lattice. Similarly to copper oxides superconductors [Bourges 21], closed loop currents create orbital magnetic moments pointing perpendicularly to the hexagonal plane. The orbital magnetic moments could be detected by polarized neutron diffraction. A structure factor calculation suggests magnetic intensity at different points in Q-space depending of correlations between loop currents in neighboring unit cells. Two situations might occur: i) if the pattern is the same in the next unit cell (such as in Figure 2), intensity is expected on Bragg peaks of the hexagonal lattice. For instance, magnetic intensity is expected at Q=(1,0,0) where the nuclear Bragg spot is weak. ii) In contrast, if the CDW is modulated the interaction between units cells, magnetic intensity should occur at the M=(1/2,0,0) point where the CDW peak is showing up [Xie22]. The same way the correlations along the vanadium planes stacking could be in-phase or out-of-phase leading to magnetic contributions at L integer (L=0,1) or half-integer (L=1/2).

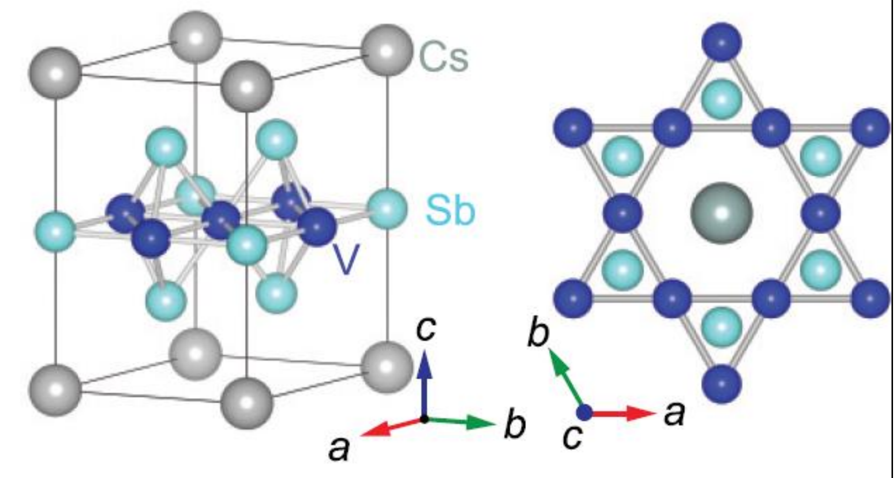

Figure 1: Hexagonal crystal structure of CsV_3Sb_5 and top view of the Kagome lattice where V atoms are in dark blue.

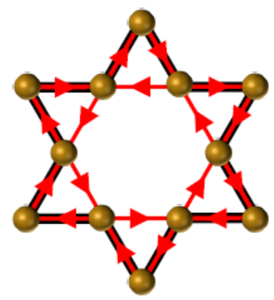

Figure 2: Orbital currents on V atoms in the Kagome lattice (from [Mielke22]).

The experiment has been performed on IN22 from 28/09/2021 to 04/10/2021. The sample was mounted in the (H,0,L) scattering plane: that was actually dictated by the sample geometry which was used in a previous experiment on IN8 to look for possible phonon softening at the CDW temperature [Xie22]. About 400 individual single crystals were co-aligned on four aluminum plates to form an assembly with a volume of 0.11 cm3 and an in-plane mosaic spread of 3.5 deg [Xie22]. The crystal assembly was put inside a He Orange cryostat and oriented in the [*H,* 0*, L*] horizontal scattering plane where the (H,0,L) Bragg spots were accessible as well as the M points (H+0.5,0,L). The polarization analysis was performed using CRYOPAD. We measured spin-flip and non-spin-flip scattering to identify possible magnetic contributions at H integer and half-integer and for L=0,1 or L=1/2.

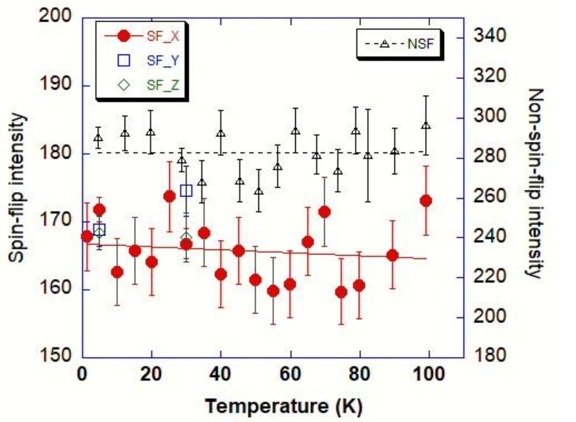

Figure 3: Temperature dependence of The Bragg peak Q=(1,0,0) of both spin-flip with the three XYZ polarizations (left scale) and non-spin-flip (right scale) intensities.

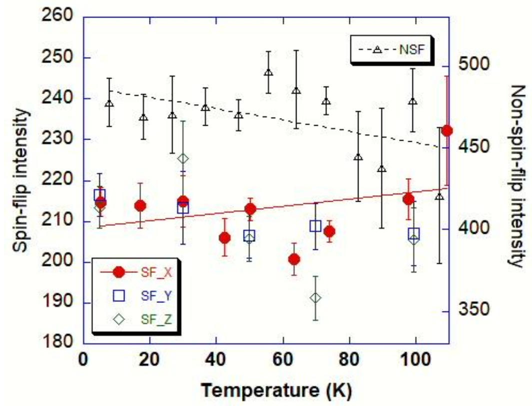

Figure 4: Temperature dependence of The Bragg peak Q=(0.5,0,0) of both spin-flip with the three XYZ polarizations (left scale) and non-spin-flip (right scale) intensities.

Figure 3 shows the temperature dependence of both spin-flip and non-spin-flip intensities at the weak nuclear Bragg peak Q=(1,0,0). No sizeable additional intensities are observed at low temperature compared to 100K (above the CDW ordering temperature of about 94K in that sample [Xie22]) in the spin-flip channel, in agreement with the polarization analysis where also no difference of intensities is observed between the three different polarization directions, XYZ. Figure 4 shows the temperature dependence of both spin-flip and non-spin-flip intensities but the M-point Q=(0.5,0,0) the wavevector where the CDW is setting up. We recently observed a weak nuclear contribution in that sample with unpolarized neutron at Q=(3.5,0,0) below T_{CDW} [Xie22]. Here, again no magnetism occurs although it is expected from the chiral flux phases [Lin21]. Other wavevectors like (1,0,1), (1,0,1/2), (1/2,0,1) and (1/2,0,1/2) were also measured using XYZ polarization analysis. No magnetism was evidenced at any of these momenta.

As there is no Bragg peak at these positions or a weak one at Q=(1,0,0), the accuracy of the measurements is quite good. Typically, the experiment accuracy was such that the moment should be lower than 0.01 or 0.02 μ_B per vanadium triangle depending of which models and form factors one may consider.

In conclusion, we have not observed so far indication of time-reversal breaking with a polarized neutron diffraction experiment in the Kagome superconductor CsV_3Sb_5 at any temperature and particularly below the CDW temperature. The measurements were done in a single scattering plane (H,0,L). Of course, other in-plane momentum directions such as (H,H,0) should be studied to address the issue and finalize that project.

References:

[Bourges21] Ph. Bourges, D. Bounoua, Y. Sidis Comptes Rendus. Physique, 22(S5) (2021) 7-31.
[Feng21] Xilin Feng, et al, Sience Bulletin 66, 1384-1388 (2021).
[Li21] H. X. Lin, et al., Phys. Rev. X, Phys. Rev. X 11, 031050 (2021).
[Lin21] Yu-Ping Lin and Rahul M. Nandkishore, Phys. Rev. B 104, 045122 (2021).
[Mielke22] C. Mielke, et al., Nature 602, 245-250 (2022).
[Xie22] Yaofeng Xie, Yongkai Li, Philippe Bourges, Alexandre Ivanov, Zijin Ye, Jia-Xin Yin, M. Zahid Hasan, Aiyun Luo, Yugui Yao, Zhiwei Wang, Gang Xu, and Pengcheng Dai, Phys. Rev. B **105**, L140501 (2022)
[Yu21] L. Yu et al., preprint, (2021), available at https://arxiv.org/abs/2107.10714