Experimental report

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Proposal: 4-02-521 **Council:** 4/2017

Title: Single-ion anisotropy in SrFe2As2

Research area: Physics

This proposal is a new proposal

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Samples: SrFe2As2

Instrument	Requested days	Allocated days	From	To
IN20 CPA	6	6	29/03/2018	05/04/2018

Abstract:

The static antiferromagnetic order as well as the magnetic excitations in doped iron-based superconductors display a remarkable anisotropy, which is inherited from their corresponding undoped parent compounds. For BaFe2As2 the single-ion anisotropy was determined by polarized inelastic neutron scattering revealing the astonishing fact that it is easier to rotate the spin out of the FeAs-layers than within. Due to the great relevance of magnetic anisotropy in Fe-based superconductors and due to the persisting controversy about the origin of longitudinal excitations we consider it important to study the magnetic anisotropy in a second undoped compound, SrFe2As2, for which unpolarised neutron scattering found significant differences.

Single-ion anisotropy in $SrFe_2As_2$

D. Gorkov, M. Braden, F. Waßer, C.-H. Lee

In iron-based superconductors there is strong interplay between the lattice, magnetism and superconductivity (SC) [1,2]. The structural distortion clearly is related to the lifting of the orbital degeneracy, but whether magnetism is driving the structural distortion (or nematicity) or whether it is just the opposite remains matter of controversy [2-9]. The magnetic anisotropy can be most easily accessed in the undoped AFM parent compounds, where static ordered moments point along the in-plane component of the propagation vector. In a layered material, one would expect an easy-plane anisotropy parallel the layers; however it turns out that the magnetically hardest axis lies in the planes perpendicular to the ordered moment. The orbital ordering thus results in a strong single-ion anisotropy breaking tetragonal symmetry [10], which reflects the nematic or orbital character of the AFM phase. More recently, an AFM phase with moments pointing out of the layers has been realised in *AE*Fe_2As_2 (*AE* = Ba, Sr) upon hole-doping at the *AE*-side [3,11-13]. For a number of compounds there is a second AFM transition at $T_{reo} < T_{SDW}$ where the moments reorient out of the layers [3,11-13]. The two directions, along which moments align in the AFM ordered states, thus perfectly correspond to the two softer axes of pure $BaFe_2As_2$. This effect documents the remarkably strong in-plane spin-space anisotropy due to spin-orbit coupling (SOC). Qualitatively the same spin-space anisotropy with two soft magnetic directions remains visible in the spin resonance mode, which develops in the superconducting state below T_c [4,14].

However, only a single undoped compound has been studied so far by polarized INS, $BaFe_2As_2$. We therefore wanted to determine the spin-space anisotropy in another undoped material, $SrFe_2As_2$. The polarized INS data for $BaFe_2As_2$ clearly show two distinct gaps for the two spin-polarization directions, of 12meV and 19meV for out-of-plane and transversal in-plane directions, respectively. This translates into single-ion anisotropy energies of the order of one meV [10], which are implied by the microscopic spin-orbit coupling [10]. For $SrFe_2As_2$ triple-axis [15] and TOF [16] experiments were interpreted by a single anisotropy gap of only 6.5meV. In addition the previous INS experiments on $SrFe_2As_2$ have been interpreted by a large dispersion perpendicular to the planes [15,16].

We mounted ~1g of single crystalline $SrFe_2As_2$, $T_S=T_N=202K$ (3 large crystals), in the [110]/[001] scattering geometry and define the frame of the polarisation analysis as the following: **Q** parallel **x**, **y** in the scattering plane but perpendicular to **x**, and finally **z** perpendicular to **x** and **y** and thus parallel to [1,-1,0]. We first analysed the magnetic Bragg peak (0.5, 0.5, 3) as function of temperature, see Fig. 1, observing the signal entirely in the $M_{a,c}$ channel in agreement with the in-plane magnetic structure (moment along a).

We mapped the spin-space anisotropy in $SrFe_2As_2$ at Q = (0.5, 0.5, L) with L = 1, 3 and 5 up to 20meV as phonon contaminations became to harmful at higher energies. Two values of the finite neutron momentum were used in order to obtain a comprehensive data set, see Fig. 2, 3 and 4. The results are very similar to those obtained for the Ba compound and clearly exclude the interpretation deduced from unpolarised experiments. c-polarized magnetic fluctuations exhibit a low-energy peak indicating a gap of 9.7(8) meV compared to 11.6meV in $BaFe_2As_2$. This can be best studied at L=1. The b polarised magnon modes – requiring a larger L value - exhibit a gap of 22.3 versus 18.9 meV in $BaFe_2As_2$. Again there is very little difference between the Sr and Ba materials. We have also studied the temperature dependence which turned out to be very small, even at T=199K slightly below the Néel ordering almost the same results were

obtained. This absence of pronounced temperature dependence seems to be related to the particularly sharp rise in the elastic intensity following the square of the magnetic moment. We found no evidence for a longitudinal mode around 20meV.

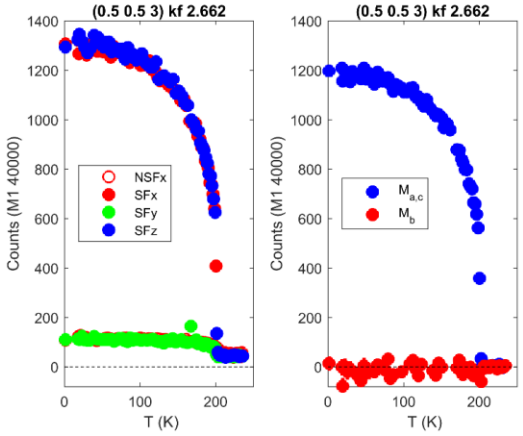

FIG. 1 : Polarization analysis of the (0.5 0.5 3) reflection on IN20. All the static signal goes into the $M_{a,c}$ component as expected. The small SF_y signal stems from the finite though quite large Flipping ratio of ~25 (determined at (112)).

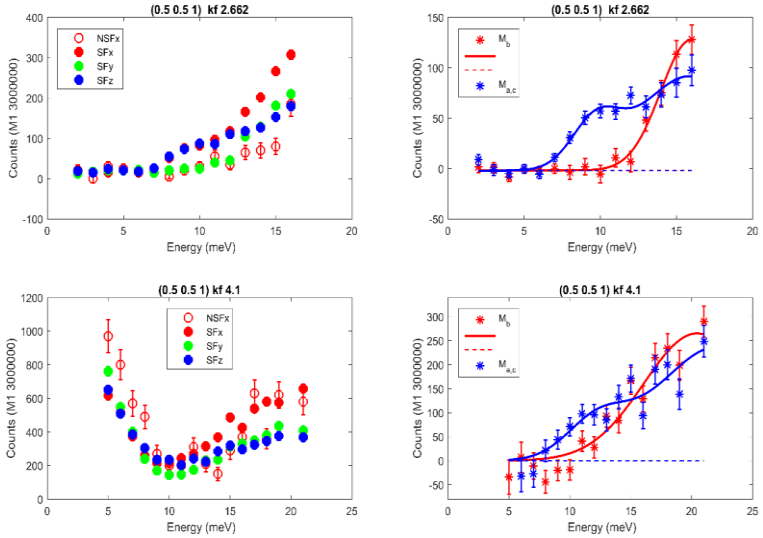

FIG. 2 : Polarization analysis of the inelastic scattering at the (0.5 0.5 1)-*Q* values with both k_f values. c-polarized magnetic fluctuations exhibit a low-energy peak indicating a gap of 9.7(8) meV compared to 11.6meV in $BaFe_2As_2$.

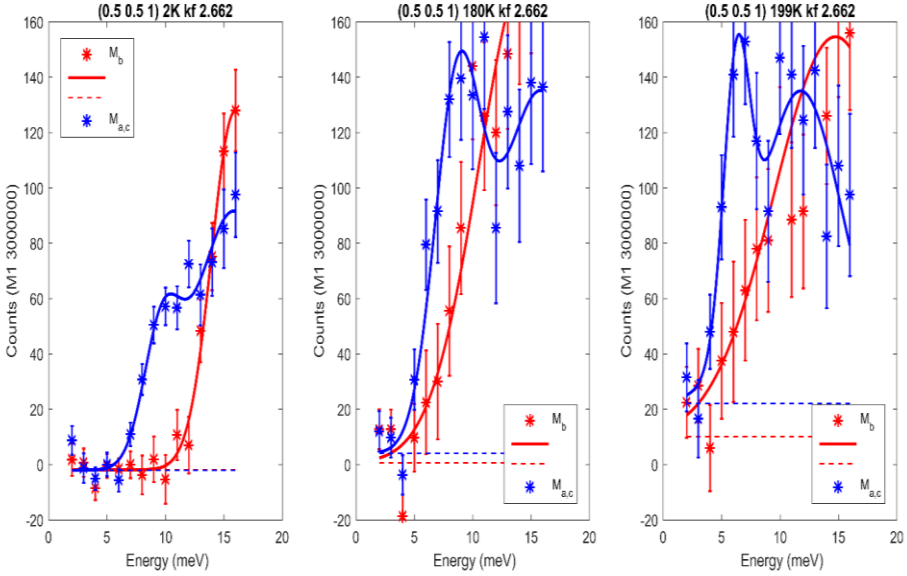

FIG. 3 : Temperature dependence of the polarized signals at (0.5 0.5 1). The gap in c-polarized magnetic fluctuations only modestly decreases upon approaching the Néel temperature. The b polarized excitations also soften or become broader in energy.

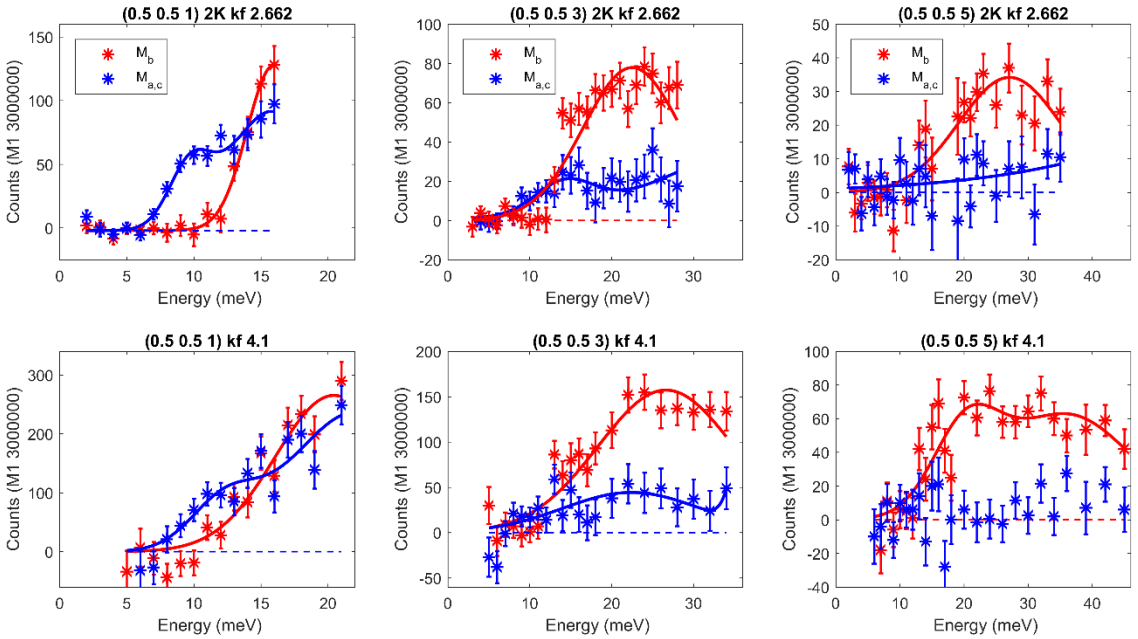

FIG. 4: Comparison of the three l values studied with two final energies. In the $M_{a,c}$ component at l=5 one would expect the longitudinal (a-polarized) excitations, but there is no evidence for a sizeable contribution near 20meV. The higher (b polarized) gap is best visible at (0.5 0.5 3) with the smaller final energy.

Conclusions

The IN20 experiment on the magnetic excitations in $SrFe_2As_2$ was quite successful producing a lot of new results. There is less difference between the Ba and Sr compounds than suggested by the unpolarised data proposing 6.5meV as spin gap. The lower gap is only slightly lower compared to the spin gaps in $BaFe_2As_2$ (9.7 versus 11.6meV) in agreement with the spin-reorientation transition that appears more stable in the Sr/Na series. For the upper gap (22.3 versus 18.9 meV) again little difference is found in the polarized INS experiments. The anisotropy in 122 materials seems thus to be little composition dependent and can therefore be considered as being a generic property.

The sharp rise of magnetic intensity is remarkable, which translates to the small suppression of the gap values upon heating. In consequence the magnetic interaction parameters including single-ion anisotropy do not essentially change with temperature. There is no evidence for a sizeable longitudinal excitation, shedding further doubt on the interpretation suggested for the Ba compound.

[1] G. R. Stewart Rev. Mod. Phys. 83, 1589 (2011) **[2]** Fernandes, R. M. et al. *Nat. phys.*,10, 97 (2014) **[3]** F. Waßer *et al.*, Phys. Rev. B 91, 060505(R) (2014) **[4]** P. Steffens *et al.*, Phys. Rev. Lett. 110, 137001 (2013) **[5]** N. Qureshi *et al.*, Phys. Rev. B 90, 100502 (2014) **[6]** C.-H. Lee et al., Phys. Rev. Lett. 111, 167002 (2013) **[7]** J.-H. Chu *et al.*, science 329, 824 (2010) **[8]** M. Nakajima et al., PNAS 108, 12238 (2011) **[9]** S. Kasahara et al. nature 486, 383 (2012) **[10]** N. Qureshi *et al.*, Phys. Rev. B 86, 060410 (2012) **[11]** L. Wang *et a*l., Phys. Rev. B 93, 014514 (2016) **[12]** A. E. Böhmer *et al.*, nat. Com. 6, 7911 (2015) **[13]** K. M. Taddei *et al.*, Phys. Rev. B 93, 134510 (2016) **[14]** F. Waßer et al., scientific reports **7**, 10307 (2017) **[15]** J. Zhao et al., PRL 101, 167203 (2008). **[16]** R. Ewings PRB 83, 214519 (2011).