Experimental report

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Council: 4/2015

Title: Magnetic excitations in Co-doped LiFeAs

Research area: Physics

This proposal is a new proposal

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Samples: Co-doped LiFeAs

Instrument	Requested days	Allocated days	From	To
IN8	7	7	15/10/2015	22/10/2015

Abstract:

LiFeAs is a special member of the iron-based superconductors, because there is so far no experimental indication of a structural or magnetic phase transition like in other FeAs parent compounds. Furthermore, the incommensurate magnetic response seems more complex for it arises from at least two different nesting mechanisms. In addition, several theory groups tried to calculate that response but arriving at contradictory results. In order to deepen the clearly insufficient understanding of the magnetic response in LiFeAs we propose to study Co-doped LiFeAs. The incommensurate magnetic excitations as function of Co doping will yield valuable information about the Fermi-surfaces and the question which hole pockets actually are involved in the magnetic fluctuations.

Experimental Report 4-02-458:
Magnetic excitations in Co-doped LiFeAs

LiFeAs is a special member of the iron-based superconductors, because there is so far no experimental indication of a structural or magnetic phase transition like in other iron-based superconductor (FeSC) parent compounds. Furthermore, the magnetic excitations are already transversal incommensurate, which indicates that LiFeAs behaves essentially as an electron-doped compound [1]. However, the incommensurate magnetic response seems more complex and two different nesting mechanisms were proposed [2]. In addition, several theory groups tried to calculate the response and the superconducting gap function, but arrive at contradictory results. The aim of the experiment is to deepen the understanding of the incommensurate magnetic response by further electron-doping, i.e. substitution of Fe by Co. Therefore, high quality single crystals with 18% Co-doping were prepared at the IFW in Dresden. Note that superconductivity for this doping level is entirely suppressed [3]. We co-aligned 4crystals with a total mass of 800mg. Due to the severe air sensitivity, the samples were constantly kept in a sealed aluminium can with Ar-atmosphere. Therefore, the sample-can exceeds the diameter of 49mm of the usual cryostat and we used a cryostat with 70mm diameter. In our previous experiment on pure LiFeAs we showed that there is no considerable dispersion of magnetic excitations along the c-direction [1] and we therefore chose the [100]/[010] scattering geometry. We used standard PG monochromator and analyser and fixed k_f to 2.662Å^{-1}.

At the beginning of the experiment we performed transversal scans along the (h,-h,0)-direction at different energy transfers in order to map the incommensurate magnetic response. Unfortunately we had to realise that the low-energy excitations, in particular with 4meV energy transfer are dominated by a signal, which can solely be traced back to the variation of the A4 angle, the secondary spectrometer arm. At higher energy transfers, e.g. 8meV, we observe a clear, but commensurate peak, cf. figure 1. This is contrary to our initial expectation, because the incommensurability in pure LiFeAs behaves like an electron-doped FeSC and we expected that a further addition of electrons would increase the incommensurability. In order to rule out that the peak is only an artefact stemming from the variation of the A4 angle, we repeated the scan in a different Brillouin zone, centred at (1.5, 0.5), although the signal would be two-times weaker due to the magnetic formfactor dependence. However, in all scans with different energy transfers the right-hand-side is strongly contaminated. Figure 2 shows an example with 10meV energy transfer. In order to check, whether all inelastic scans where affected by some contamination we checked the phonons with 6meV energy transfer, cf. figure 3. Because the phonons look fine, we changed to the Si-monochromator and repeated the scans from the beginning. This caused a reduction of the incoming flux by a factor two at least and did not yield an improvement at all, unfortunately. Therefore we went back to the PG monochromator and changed k_f to 4.1Å^{-1}. But also in this configuration the data does not become any cleaner. Finally, we returned to the initial condition with k_f = 2.662Å^{-1} and performed rocking scans with |Q| = |(0.5 0.5 0)| and various energy transfers. The rocking scans are almost parallel to the (h,-h,0) scan-direction in this Brillouin zone. The advantage is, that the A4 angle is constant during the scan and cannot produce any artefacts. Figure 4 depicts such a rocking scan with 8meV energy transfer. Surprisingly the magnetic response is commensurate. We also repeated the rocking scans in the next Brillouin zone, centred at (1.5 0.5). Note that in this zone the trajectory of the rocking scans displays a strong deviation from the transversal scan along (h, 2-h)-direction. Although these scans cannot harden the idea that the magnetic response shifts from incommensurate to commensurate at 18% Co-doping, they can at least show that real signal can be found in the next Brillouin zone. Figure 5 presents such a rocking scan with |Q| = |(1.5 0.5 0)| and 8meV energy transfer. Moreover, we performed several rocking scans in both Brillouin zones (BZs) and fitted the data by Gaussians on a linear sloped background. The extracted amplitude was normalised by the magnetic formfactor and is summarised in figure 6. The signal in both BZs is consistent and the overall energy dependence can be described by a single relaxor function yielding a damping $\Gamma = 8.1(1.2)$meV. Finally, we repeated the rocking scans in the first BZ at different temperatures with 8meV energy transfer and observed simultaneous decrease of the amplitude and an increase of the width, as it is expected for magnetic excitation, cf. insets figure 4.

In conclusion our experiment finds that magnetic scattering in 18% Co doped LiFeAs is significantly weaker than that in the pure material, and the character changes from incommensurate in pure LiFeAs to commensurate scattering centred at (0.5 0.5 0).

[1] N. Qureshi et al., PRL 108, 117001 (2012) **[2]** N. Qureshi et al., PRB 90, 144503 (2014) **[3]** Z. R. Ye et al., PRX 4, 031041 (2014)

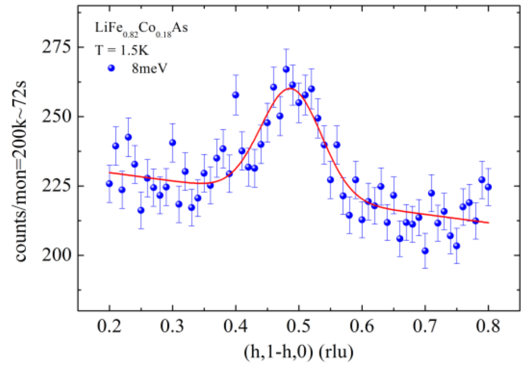

Figure 2Transversal scan at 1.5K with 8meV energy transfer displaying a single commensurate peak. The data is fitted by a Gaussian on a linear slope.

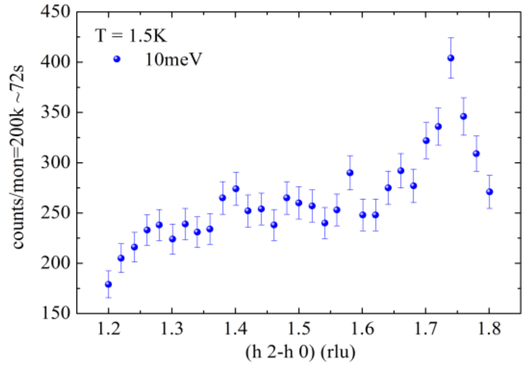

Figure 1 Transversal scan in the BZ centred at (1.5 0.5) with 10meV energy transfer. The right-hand-side is strongly contaminated.

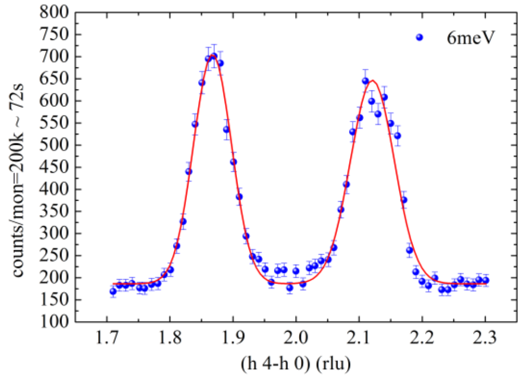

Figure 4 Constant energy scan through the phonon branches centred at (2 2 0) with 6meV energy transfer. The phonons are fitted by two Gaussians.

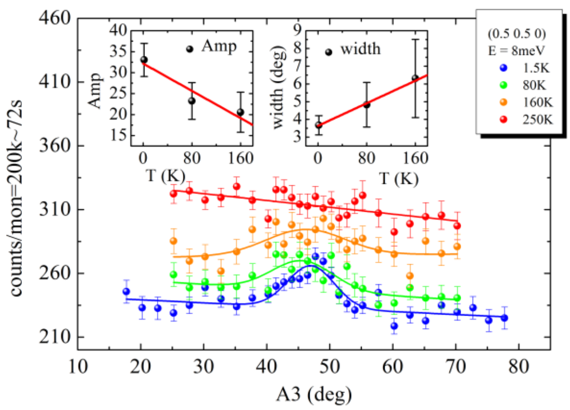

Figure 3 Rocking scans with |Q| = |(0.5 0.5 0)| and 8meV energy transfer at different temperatures. The left inset shows the decrease of the amplitude, while the inset on the right depicts the increase of the width.

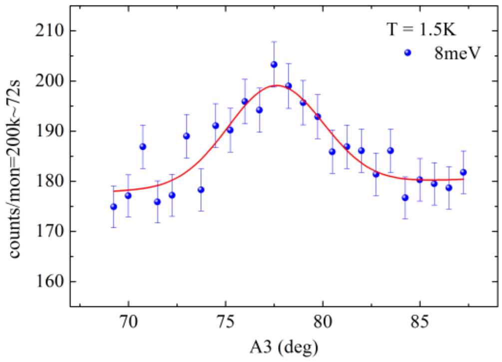

Figure 5 Rocking scan with |Q| = |(1.5 0.5 0)| and 8meV energy transfer at 1.5K. The signal is described by a Gaussian on a linear background.

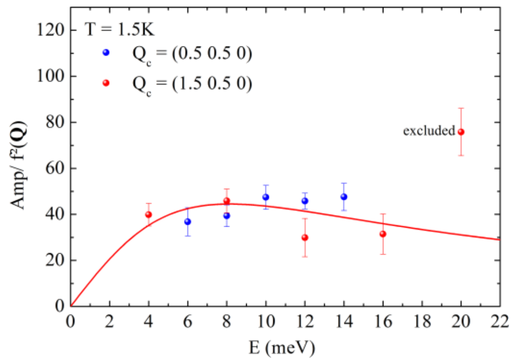

Figure 6 Summary of the extracted and normalised by the magnetic formfactor amplitudes from the rocking scans in two different BZs. The solid line is a single relaxor fit, but the point at 20meV has been excluded.