# Experimental Report

29/01/2015

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| **Proposal:** | **4-01-1372** | **Council:** | 4/2014 | |
| **Title:** | Spin gaps in heavily overdoped BaFe2-xNixAs2 | | | |
| **This proposal is a new proposal** | | | | |
| **Research Area:** | Physics | | | |
| **Main proposer:** | **LUO Huiqian** | | | |
| **Experimental Team:** | LUO Huiqian<br>LIU Zhaoyu | | | |
| **Local Contact:** | IVANOV Alexandre | | | |
| **Samples:** | BaFe2-xNixAs2 | | | |

| Instrument | Req. Days | All. Days | From | To |
|---|---|---|---|---|
| IN8 Flatcone | 8 | 8 | 10/10/2014 | 18/10/2014 |

**Abstract:**

A direct correlation between spin excitations and superconductivity in iron-based superconductors is the evolution of low energy spin excitations in the over-doped region.In BaFe2-xNixAs2 system, the low energy spin excitations decreased significantly upon Ni doping, and finally form a large spin gap up to 50 meV in the heavily over-doped non-superconducting BaFe1.7Ni0.3As2. While neutron scattering on the overdoped BaFe1.82Ni0.18As2 with Tc=8 K suggests that the low energy spin excitations persist to 5 meV at least. But it is still not clear for the formation of large spin gap in overdoped samples and whether it is related to the disappearance of superconductivity in overdoped regime. Therefore, we propose to do inelastic neutron scattering measurements on the heavily overdoped BaFe2-xNixAs2 around the superconducting zone boundary, mainly focusing on the low energy spin gaps. A comprehensive determination of spin gaps through the whole phase diagram will give us important information concerning the relationship between low energy spin excitations and superconductivity.

# Experiment Report of Proposal 4-01-1372

## Spin gaps in the heavily overdoped $BaFe_{2-x}Ni_xAs_2$

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In iron pnictides, high temperature superconductivity is associated with both the presence of high-energy spin excitations and a coupling between low-energy spin excitations and itinerant electrons [1]. Particularly in the electron doped $BaFe_{2-x}Ni_xAs_2$ system, the low energy spin excitations decrease significantly upon Ni doping, and finally form a large spin gap up to 50 meV in the heavily over-doped non-superconducting $BaFe_{1.7}Ni_{0.3}As_2$ [2], while our previous neutron scattering experiments on overdoped superconducting $BaFe_{1.82}Ni_{0.18}As_2$ suggest that the low energy spin excitations persist to 3 meV at least [3]. So far, it is still not clear for the formation of large spin gap in overdoped samples and whether it is related to the disappearance of superconductivity in overdoped regime, where the hole pockets are eliminated near the zone boundary of superconductivity [4]. Our proposed experiment is focusing on the doping evolution of low-energy spin excitations for heavily overdoped $BaFe_{2-x}Ni_xAs_2$ system.

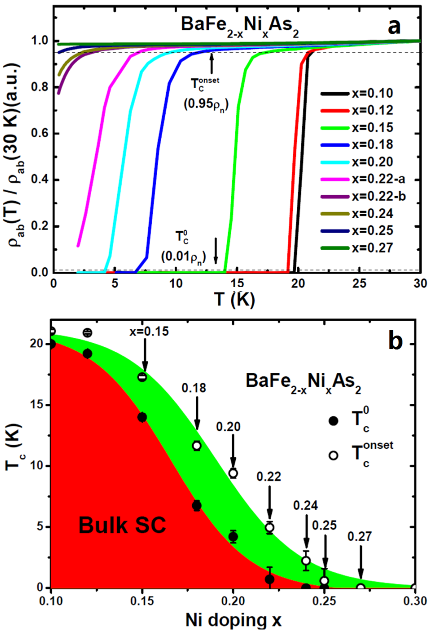


Fig. 1 Superconducting transition and phase diagram of heavily overdoped $BaFe_{2-x}Ni_xAs_2$.

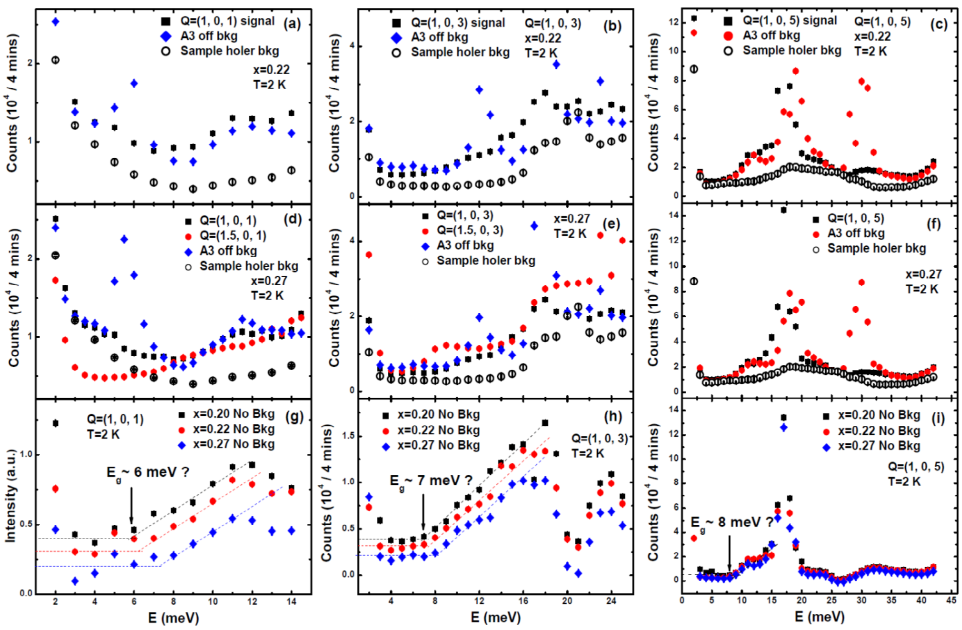


Fig. 2 Energy dependence of spin excitations and background in overdoped $BaFe_{2-x}Ni_xAs_2$.

The superconducting transition and phase diagram of overdoped $BaFe_{2-x}Ni_xAs_2$ is shown in Fig. 1, where the zone boundary for full superconductivity down to 0 K is x=0.25. Since we have already measured three dopings x=0.15, 0.18 and 0.30, we plan to further measure x=0.20, 0.22, 0.25 and 0.27 in this experiment. Due to the limitation of beamtime, we actually measured three dopings with x=0.20, 0.22 and 0.27. For each doping, we co-aligned about 20 grams of single crystals on 5 thin aluminum plates by hydrogen-free glue in scattering plane [H, 0, L] with orthorhombic lattice parameters a=b=5.57 Å, c=12.86 Å . The final energy was fixed at $E_f$=14.87 meV, with pyrolytic graphite as the monochromator, analyzer, and filters.

We did energy scans up to 45 meV to search for magnetic signal centering at Q=(1,0,1), (1,0,3) and (1,0,5). To determine the spin gaps, one should find reliable backgrounds comparing to the magnetic signals. We tried three methods for background scans: (1) Energy scans at Q=(1.5, 0, 1) and (1.5, 0, 3) away from the peak center (red dots in Fig. 2(d) and (e)); (2) Energy scans at the same momentum transfer after rotating A3 (Theta) 45 degrees off (blue diamonds in Fig. 2 (a)(b)(d)(e)); (3) Energy scans at the same momentum transfer on the empty aluminum sample holder (open circles in Fig. 2(a)-(f)). However, due to rather weak magnetic signals in these compounds and multi-scattering at low angle of A4, it hard to find any clear difference between magnetic signal and backgrounds in methods (1) and (2). Moreover, more troubles are introduced by the spurious signal from Bragg scattering of high order neutrons with wavelength λ/n, and the aluminum phonon signal from sample holder. Roughly, we subtracted the data by identical scans on empty sample holder and found the spin gaps are about 6 meV for Q=(1,0,1), 7 meV for Q=(1,0,3) and 8meV for Q=(1,0,1), respectively, while no significant doping dependence was found. These results, however, are neither we expect, nor consistent with previous results. Indeed, we performed some typical Q scans at E=5, 9, 15, 20 meV and found the signal is far away from standard Gaussian distribution (Fig. 3), they are probably mixed with incoherent scattering signal and spurious signal from Bragg scattering and phonons. In summary, we may find spin gaps about 6 - 8 meV in overdoped $BaFe_{2-x}Ni_xAs_2$, but more experiments are definitely needed to be done to fully clarify this issue. One better way to solve this problem is experiment by polarized neutron beam, which will eliminated the mixed spurious signal from nuclear scattering and give much clean background.

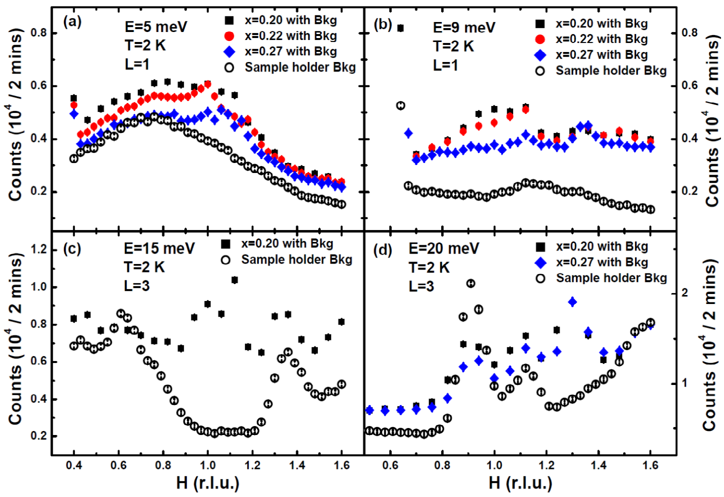

Fig. 3 Constant-energy scans at 5, 9, 15, 20 meV for heavily overdoped $BaFe_{2-x}Ni_xAs_2$, where open circles are identical scans for aluminum sample holder.

References:

[1] P. Dai, J. Hu and E. Dagotto, Nature Phys. 8, 709 (2012).

[2] M. Wang *et al.*, Nature Commun. **4**, 2874(2013);

[3] H. Luo *et al.*, Phys. Rev. B **88**, 144516 (2013);

[4] C. Liu *et al.*, Phys. Rev. B **84**, 020509(R) (2011); S. Ideta, *et al.*, Phys. Rev. Lett.,**110**, 107007 (2013);