

# Competition between magnetism and superconductivity in underdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$

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The discovery of superconductivity in the iron pnictide compounds has created tremendous excitement in the scientific community as these compounds provide another fascinating opportunity to study the subtle aspects of interactions between superconductivity, magnetism, and structure. The parent compounds of the 122 family ( $\text{AFe}_2\text{As}_2$ , A = Alkaline earth) undergo transitions from a high-temperature paramagnetic tetragonal phase to a low temperature antiferromagnetic (AF) orthorhombic structure [1]. Doping either holes or electrons into the system will suppress both the AF and structural transitions and lead to superconductivity [1]. In the underdoped electron-doped (Co or Ni) samples where the antiferromagnetism (AF) and superconductivity coexist, the AF order will be slightly suppressed below  $T_c$  but no obvious structural change is observed, as shown in Fig. 1 [2]. Neutron powder diffraction [3] and other experiments [4] suggest that the coupling among the AFM, structure and superconductivity may be stronger in the K-doped (hole-doped) 122 system but no neutron diffraction study has been performed on these single crystals.

We used C5 triple axis spectrometer to study single crystals of  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$  with  $x = 0.12$  ( $T_c = 0$ ), 0.20 ( $T_c = 28$  K) and 0.25 ( $T_c = 32$  K) with neutrons. To ensure that the higher order neutron contamination was minimized especially when antiferromagnetic peaks were measured, we used two PG filters in the  $k_f$  side with a wavelength of 2.37 Å ( $E_f = 14.56$  meV). The nuclear structural peaks were measured with  $\lambda = 3$  Å neutrons without PG filter.

We found that the non-superconducting  $x = 0.12$  sample shows similar qualitative AFM properties to that of the parent compound  $\text{BaFe}_2\text{As}_2$  albeit with a reduced  $T_N$ . The magnetic peaks remain resolution limited, i.e. the magnetic correlations remain infinite similar to the parent compound. This suggests that for low enough

doping the nature of the AFM is not changed and only  $T_N$  is reduced.

However, for  $x = 0.25$  sample, we found that the magnetic and nuclear structures are strongly coupled to superconductivity. Fig. 2a and 2b show the temperature dependence of the peak intensity at the AF wave vector (0.5, 0.5, 3) and the full-width-at-half-maximum (FWHM) of the (1, 1, 0) nuclear peak respectively. Since the tetragonal-orthorhombic structural phase transition can be probed via the splitting of the (2, 2, 0) nuclear Bragg peak, the difference between a and b lattice constants can be inferred from the value of the FWHM of the (1, 1, 0) peak measured with  $\lambda/2$ . The magnetic intensity observed at (0.5, 0.5, 3) drops to a constant value above 73 K indicating  $T_N = 73$  K. Our measurements of the FWHM of the (1, 1, 0) peak also indicates that it drops to a constant value above 73 K. These suggest that the sample has a tetragonal structure without long-range AF order above 73 K. The system enters into the AFM state along with a structural change at 73 K as evident by the increase of the FWHM of the (1, 1, 0) peak. The magnetic peaks remain resolution limited. The magnetic intensity increases with decreasing temperature but drops suddenly at  $T_c$  on cooling. After reaching its minimum at 28 K, the intensity of the (0.5, 0.5, 3) increases with decreasing temperature again. Meanwhile, the FWHM of the (1, 1, 0) peak shows similar changes to the magnetic intensity suggesting the difference between a and b lattice constants is directly coupled to the strength of the AFM.

Similar temperature dependences were also observed for  $x = 0.20$  sample for both magnetic and nuclear peaks however the changes below  $T_c$  were less pronounced compared to the  $x = 0.25$  sample.

Our results suggest that the coupling between magnetic and nuclear structures as well as superconductivity in

hole-doped  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$  is much stronger than that in the electron-doped  $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$  or  $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ . Further investigation is required to identify whether such differences come from the different types of doping (hole/electron) or doping at different atomic positions (Ba vs. Fe site).

#### References

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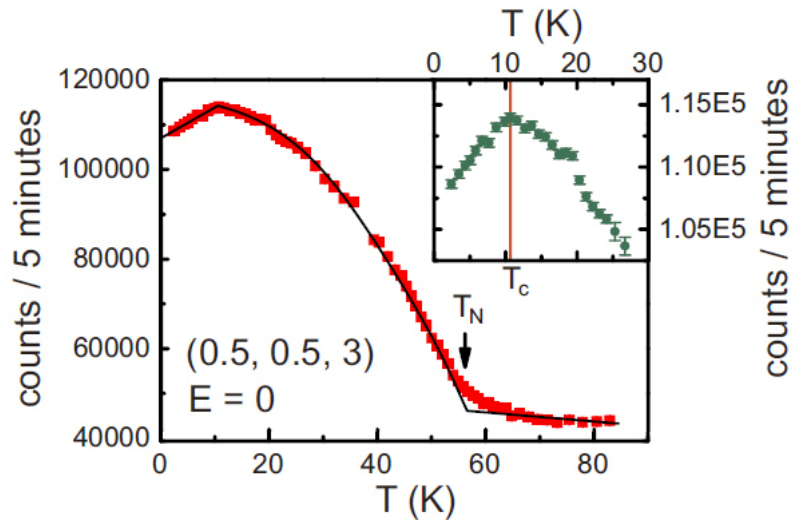


Fig. 1 Temperature dependence of the AF peak (0.5, 0.5, 3) in  $\text{BaFe}_{1.925}\text{Ni}_{0.075}\text{As}_2$  [2].

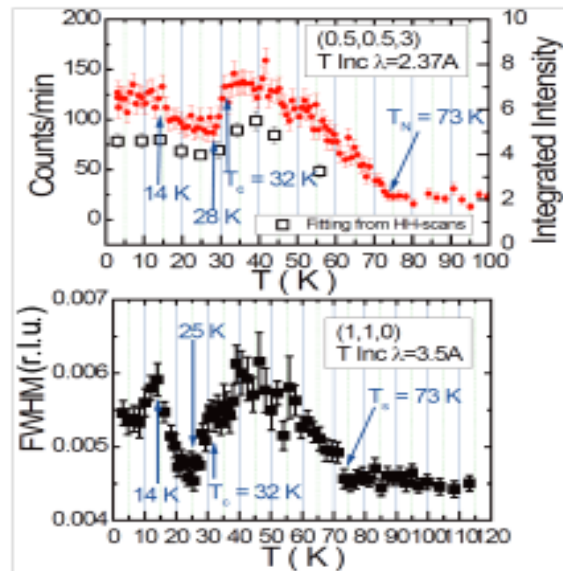


Fig. 2 Temperature dependence of (a) the AF (0.5, 0.5, 3) peak intensity and (b) the FWHM of the (1, 1, 0) structure peak.