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Detailed microscopic investigation of $BaFe_2As_2$ single crystals

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Abstract

Although it has been previously reported that $BaFe_2As_2$ has a single transition (structural and magnetic happening simultaneously) at $T_0 \cong 138K$, investigating deeper in that direction we perceive that a splitting happens in the pure sample. The structural transition (tetragonal → orthorhombic) has a higher characteristic temperature, suggesting a relation between the lattice organization and the behavior of the spins, and therefore, with the antiferromagnetism (AFM) and superconductivity (SC).

Key words: nuclear magnetic resonance, iron-based superconductors, pnictides

Introduction

Iron-based superconductors have been deeply studied because of their relatively high superconducting temperatures T_c and their relevance to shed new light to our understanding about unconventional (non-BCS) superconductivity. The $BaFe_2As_2$ single crystals investigated in this work were prepared using the In-flux growth technique and characterized through specific heat, resistivity, X-ray diffraction and Nuclear Magnetic Resonance (NMR). So far, many reports suggest that this material undergoes a structural (tetragonal to orthorhombic) transition simultaneously with an AFM (spin density wave) one at about $T_0 \cong 138K$. Nonetheless, when iron ions are substituted by Co, Cu, Mn or Ni, such a transition actually splits into two. For the doped $BaFe_2As_2$ it is well known that the structural transition occurs prior to the AFM long range order. Here we claim that these transitions can also be distinguishable for the undoped $BaFe_2As_2$ when it is grown by In-flux method within a finite temperature range in clear contrast with what have been previously reported.

Results and Discussion

Specific heat of our $BaFe_2As_2$ single crystals revealed that both transitions are discernible with $T_s > T_{SDW}$ as shown in Image 1. This fact supports the scenario where these transitions are correlated with each other and the AFM emerging as a consequence of lattice distortion due to a magneto-elastic coupling (Nematic order) between the spin and charge degrees of freedom. Other microscopic techniques such as X-ray diffraction and NMR provide further insight regarding this scenario. As one can see in the inset to Image 1, there is a region where both tetragonal (PM) and orthorhombic (AFM) phases cohabit within finite temperature range in the sample.

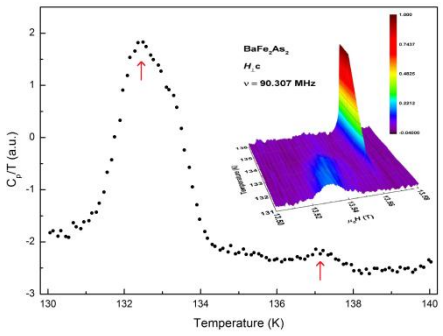

Image 1. Specific heat/temperature x temp. ($T_N \cong 133K$ and $T_S \cong 137K$). NMR on the inset

Conclusions

This detailed microscopic investigation points out that the structural (T-O) and magnetic SDW transitions observed in the iron-arsenide $BaFe_2As_2$ compound can also be distinguishable within a finite temperature range when the single crystal is grown by In-flux method which has recently proven to yield better crystallographic sample quality. This is in clear contrast with previous reported in the literature

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