Detailed microscopic investigation of BaFe$_2$As$_2$ single crystals

Thales A. Caldonazo (IC), Guilherme G. Lesseux (PG), Mario M. Piva (PG), Matheus Radaelli (PG), Camilo B. R. Jesus (PG), Dina Tobia (PQ), Eduardo G. M. Silva (PQ), Pascoal G. Pagliuso (PQ), Ricardo R Urbano (PQ).

Abstract

Although it has been previously reported that BaFe$_2$As$_2$ has a single transition (structural and magnetic happening simultaneously) at $T_0 \approx 138K$, investigating deeper in that direction we perceive that a splitting happens in the pure sample. The structural transition (tetragonal $\rightarrow$ 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$_2$As$_2$ 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 $T_0 \approx 138K$. Nonetheless, when iron ions are substituted by Co, Cu, Mn or Ni, such a transition actually splits into two. For the doped BaFe$_2$As$_2$ 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$_2$As$_2$ 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$_2$As$_2$ 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. ($T_s \approx 133K$ and $T_0 \approx 137K$). 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$_2$As$_2$ 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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