High Field NMR in Transition Metal Substituted BaFe2As2

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Introduction

The nature of the magnetic transition in iron arsenides has raised many debates among researchers. Magnetic order is preceded by a tetragonal to orthorhombic structural transition, and there is a belief that elastic degrees of freedom play an important role on the magnetism as well as superconductivity in the FeAs family [1]. This is a quite relevant issue to understand the suppression of T_N by applied pressure and/or isovalent substitution. Moreover, there is an increasing evidence that local crystal field configuration is an important factor in determining the physical properties of this family of materials. In fact, chemical substitutions do not seem to introduce extra carriers in most cases, but this remains an open question.

We have performed ^{75}As NMR experiments on transition metal substituted $BaFe_{2-x}M_xAs_2$ (M = Co, Cu). We interpret the NMR results in terms of crystal field configuration, and our data suggests a coexistence region of paramagnetic and antiferromagnetic phases.

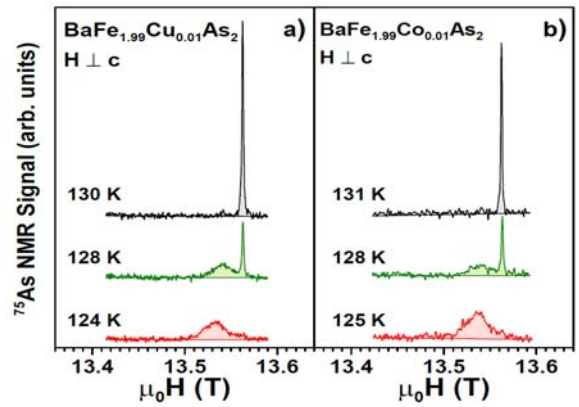

Fig. 1 ^{75}As NMR signal across the transition with magnetic field perpendicular to the *c*-axis for (a) Cu and (b) Co substituted BaFe2As2.

Experimental

$BaFe_{2-x}M_xAs_2$ (M = Co, Cu) single crystals were grown by In-flux technique. The samples were specifically selected to display the same structural/magnetic transition temperature, T_0, in order to investigate the crystal field effects in each sample. The NMR spectra were taken as field swept at fixed temperatures in the 4 K – 150 K range and magnetic fields around 13.5 T. Samples were aligned so that the magnetic field was applied either parallel or perpendicular to the crystallographic *c*-axis.

Results and Discussion

We have observed a central transition with very narrow line width, even for substituted samples (5 kHz for the pure and 9 – 15 kHz for Co and Cu, respectively), indicating high crystallographic quality. Also, our NMR data show that both Co and Cu samples present the same quadrupolar splitting (not shown). Since the samples were chosen to have the same T_0, this striking result indicates that electronic doping is not the effective mechanism but rather geometric factors of the Fe-As tetrahedral must dominate the underlying physical properties of Ba122. Finally, our NMR data suggest coexistence of tetragonal/paramagnetic (T/PM) and orthorhombic/SDW (O/SDW) phases in a 5 K range, as shown in Fig. 1. These results are in consonance with our previous investigation on K-substituted Ba122 [2].

Conclusions

Our NMR results support the high quality of our In-flux grown samples and, due to such a high quality, we have observed that the same T_N are driven by the configuration of atoms in the Fe-As plane, and that the extra carriers that might dope the material electronically in fact stay localized on the substituted atoms sites. Also, we have observed coexistence of T/PM and O/SDW phases in the same temperature range for different substituting atoms, which indicates that this is inherent to the Ba122 family. These NMR results have provided strong support to a paper [3] and are forming the basis to another yet to appear in May 2014 in the Journal of Applied Physics [4].

Acknowledgements

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References

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[2] R. R. Urbano et al., Phys. Rev. Lett. **105**, 107001 (2010).	[4] T. M. Garitezi et al., to appear in J. Appl. Phys. (2014)