A Mössbauer study of the magneto-structural coupling effect in $SrFe_2As_2$ and SrFeAsF

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Abstract In the present paper, we report a comparison study of $SrFe_2As_2$ and SrFeAsF using Mössbauer spectroscopy. The temperature dependence of the magnetic hyperfine field is fitted with a modified Bean–Rodbell model. The results give much smaller magnetic moment and magneto-structural coupling effect for SrFeAsF, which may be understood as due to different inter-layer properties of the two compounds.

Keywords Mössbauer spectroscopy · Iron based superconductors · Magneto-structural coupling effect

1 Introduction

The surprising discovery of superconductivity by Hideo Hosono and co-workers in fluorine-doped LaFeAsO with transition temperature as high as 26 K [1] has stimulated worldwide efforts to study this new family of superconductors [2]. Among many discovered iron-based superconductors, the 122-type $AeFe_2As_2$ (Ae = Ba, Sr, Ca, Eu) and the 1111-type ReFeAsO (Re = La, Ce, Pr, Nd, etc.) families are the most studied materials [2]. And it has been shown that magnetism and structural tuning may play important roles in the pairing mechanism of these superconductors [3, 4]. There is also an interesting interplay between the crystal structure and magnetism
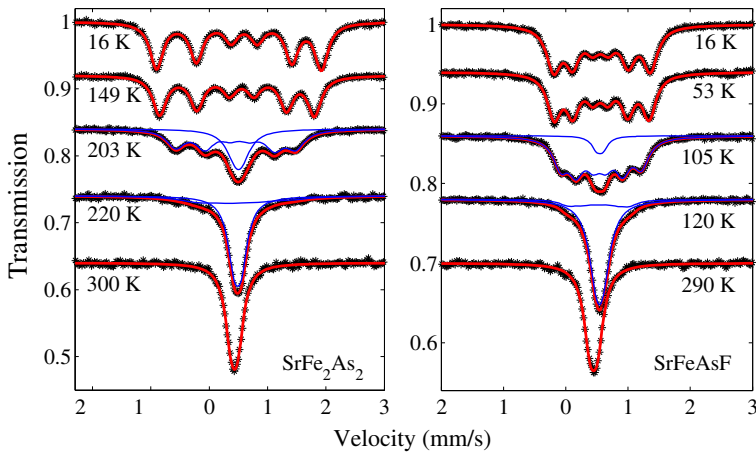
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Fig. 1 Mössbauer spectra taken at indicated temperatures of the $SrFe_2As_2$ and SrFeAsF compounds

degrees of freedom [5]. However, a clear understanding of the relationship between magnetism and structural tuning is far from reached.

Mössbauer spectroscopy has been proved to be a useful tool to probe the local magnetic field at the iron nucleus of these materials [6, 7]. A comparison study of the 122-type and 1111-type families may yield valuable information about the magneto-structural coupling effect (MSCE). Therefore, in the present work, $SrFe_2As_2$ and SrFeAsF compounds are prepared and studied through Mössbauer spectroscopy. The result suggests that the MSCE for $SrFe_2As_2$ is stronger than that for the SrFeAsF compound, which may be due to the different properties of Sr and SrF inter-layers for $SrFe_2As_2$ and SrFeAsF, respectively.

2 Experimental

Polycrystalline $SrFe_2As_2$ and SrFeAsF compounds were prepared using conventional solid-state reaction method similar to previous reports [8, 9]. Phase purity were checked by X-ray powder diffraction (XRPD) on a Philips X'pert diffractometer with Cu K_α radiation. The lattice constants were found to be $a = 3.925$ Å, $c = 12.365$ Å for $SrFe_2As_2$ and $a = 4.002$ Å, $c = 8.970$ Å for SrFeAsF, which are in good agreement with previously reported values [8, 9]. Transmission Mössbauer spectra at temperatures between 16 K and 300 K were recorded using a conventional constant acceleration spectrometer with a γ-ray source of 25 mCi ^{57}Co in palladium matrix.

3 Results and discussion

Mössbauer spectra (MS) at selected temperatures are shown in Fig. 1. As can be seen, the spectra for both $SrFe_2As_2$ and SrFeAsF compounds can be well fitted by only one doublet/(sextet) above/(below) the transition region, indicating that there is no Fe containing impurity phase in our sample, coincidence with the XRPD results.

Fig. 2 Temperature dependence of the hyperfine field, $B_{hf}(T)$, extracted from least-squares fits of the Mössbauer spectra. The *blue solid lines* are theoretical fits to the data (see text)
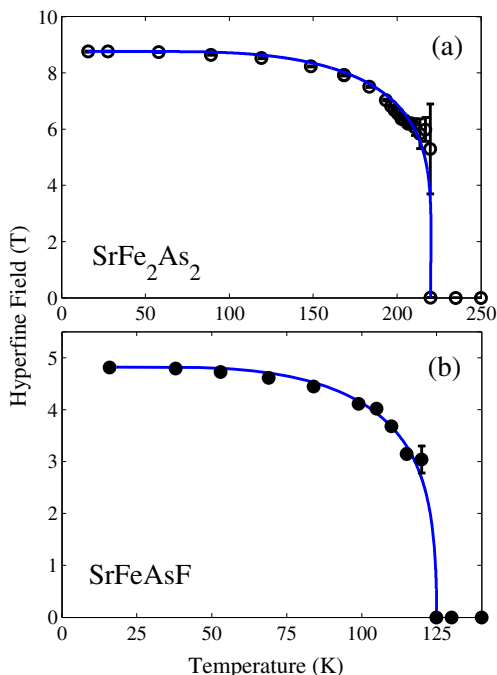
At temperatures in the transition region the MS are fitted with the superposition of a doublet and a sextet. This means that the spin density wave (SDW) develops below or about onset of the magnetism and rapidly reaches quasi-rectangular form upon lowering of the sample temperature [6].

The variation of the HF with temperature is shown in Fig. 2. To investigate the MSCE, we fit the temperature dependence of the HF with a modified Bean–Rodbell model. To include MSCE, we rewrite the Gibbs free energy per unit volume as [7, 10] $G = -\frac{1}{2}Nk_BT_Nm^2 + \frac{1}{2}B\varepsilon^2 + \lambda\varepsilon m^2 - TNk_B\left[\ln 2 - \frac{1}{2}\ln\left(1 - m^2\right) - m\tanh^{-1}m\right]$, where m is the sublattice magnetization, ε the strain, T_N the Néel temperature, B the elastic modulus, k_B the Boltzmann constant, and λ is the coupling coefficient. Following the same procedure as done by Bean and Rodbell, first minimizing the total energy with respect to ε and then with respect to m one can obtain the implicit dependence of m on T as [10] $T/T_N = \left(m/\tanh^{-1}m\right)\left(1 + \eta m^2/3\right)$, where $\eta = 6\lambda^2/T_NBNk_B$ is a fitting parameter, which involves the magneto-structural coupling coefficient and elastic modulus and controls the order of the magnetic phase transition with $\eta < 1$ for a second order phase transition and $\eta > 1$ for a first order phase transition. Obviously, a larger λ will lead to a larger η, which will creates a larger energy barrier in the free-energy landscape when $\eta > 1$ [7]. This should leads to a sharper magnetic transition as shown in Fig. 2 for SrFe₂As₂.

The fitted results are also plotted in Fig. 2 (solid curve). The zero temperature HF is found to be 8.76 T and 4.82 T for SrFe₂As₂ and SrFeAsF, respectively. And T_N is determined to be 220 K for SrFe₂As₂ and 125 K for SrFeAsF, which are in good agreement with reported values [8, 9]. The structural factor η is found to be 1.09 and 0.8 for SrFe₂As₂ and SrFeAsF, respectively, indicating stronger MSCE for

$SrFe_2As_2$ than SrFeAsF. The only difference for the two compounds is the non-superconducting layers, namely Sr layer and F-Sr-F layer for $SrFe_2As_2$ and SrFeAsF, respectively. From the XRPD results one can obtain that a larger F-Sr-F layer leads to a larger distance along the *c*-direction between the FeAs plane for the SrFeAsF, which should reduce the effective interactions between the FeAs layers. Moreover, due to different properties of Sr and F-Sr-F inter-layers for $SrFe_2As_2$ and SrFeAsF, the crystal field for the two compounds should be different. This could lead to a completely different electronic structure for the two compounds, which may lead to the observed different magnetic moments and MSCE.

4 Conclusions

In summary, our Mössbauer results show that $SrFe_2As_2$ have a much larger magnetic moment than SrFeAsF. And the antiferromagnetic phase transition is sharper for $SrFe_2As_2$, indicating a stronger magneto-structural coupling effect than that in SrFeAsF, which might due to different inter-layer properties of the two compounds.

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