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NMR Studies on Iron Pnictide Superconductors of $\text{LaFeAsO}_{0.89}\text{F}_{0.11}$ and Ca-Fe-Pt-As

Y Kobayashi^{1,3}, T Iida¹, K Suzuki¹, E Satomi¹, T Kawamata^{1,3,*}, M Itoh^{1,3}, and
M Sato^{2,1,3,#}

¹ Department of Physics, Graduate School of Science, Nagoya University, Nagoya
464-8602, Japan

² Toyota Physical and Chemical Research Institute, Nagakute, Aichi 480-1192, Japan

³ JST TRIP, Nagoya University, Nagoya 464-8602, Japan

E-mail: i45323a@cc.nagoya-u.ac.jp (Y Kobayashi)

Abstract. We first show results of $(\text{NMR}-1/T_1)\text{-}T$ curves of $\text{LaFeAsO}_{1-x}\text{F}_x$ samples with various x values. It does not have the coherence peak and absolute values of $d\log(1/T_1)/d\log(T/T_c)$ shows the dome shaped x dependence with a maximum at the optimum x value. Considering the T dependent energy broadening of quasi-particles and magnetic susceptibility below T_c , we show that the nonexistence of the coherence peak cannot necessarily be regarded as the evidence for the $S_{\pm}$ symmetry of the order parameter. We also present NMR data on the superconducting Ca-Fe-Pt-As system recently found by Kakiya *et al.* ⁷⁵As-NMR spectra taken for single crystals of the system indicate clear evidence that Pt atoms are doped into the FeAs conducting layers consistently with the results of the structure analyses, indicating that the superconductivity survives even in the existence of strong impurity scattering of the conduction electrons.

1. Introduction

To investigate whether the signs of the order parameters Δ on the disconnected Fermi surfaces around Γ and M points are same or opposite in Fe pnictide superconductors[1], we have measured various physical quantities and analyzed[2-9], impurity-doping effects on superconducting transition temperatures T_c and transport properties[2, 3, 5, 6, 8], NMR relaxation rate $1/T_1$ [4, 5, 7], and magnetic excitation spectra[9]. If the $S_{\pm}$ symmetry with sign reversal of the Δ 's[10, 11] is realized in the systems, as is widely believed, the superconducting pairing is due to the magnetic interaction. However, detailed results of the T_c suppression rate so far obtained by our group for various nonmagnetic impurities strongly indicate that the symmetry is S_{++} which does not have the sign change. Considering this result and also considering that the T_c value as high as ~ 55 K observed for Nd1111 system is difficult to be explained by the ordinary phonon mechanism, we may have to consider a new mechanism such as the one related to the orbital degrees of freedom[12].

* present address: Dept. of Phys., Grad. School Eng., Tohoku Univ., Sendai 980-8578, Japan.

present address: Research Center for Neutron Science and Technology, Comprehensive Research Organization for Science and Society, 162-1 Shirakata, Tokai, Ibaraki 319-1106, Japan.

In this paper, we present first NMR results for $\text{LaFeAsO}_{1-x}\text{F}_x$ and briefly argue on the nonexistence of the coherence peak (CP) in NMR- $1/T_1$ curves, which has been considered as the evidence for the $S_{\pm}$ symmetry, because for this symmetry, the coherence term contributing to $1/T_1$ in the superconducting state is suppressed because of the cancellation of the inter- and intra-Fermi surface scatterings. However, as we show below, the nonexistence of CP may not necessarily indicate the $S_{\pm}$ symmetry [5, 7]. Second, we present results of ^{75}As -NMR/NQR measurements on the Ca-Fe-Pt-As system newly found by Kakiya *et al.*[13]. We prepared these samples and reported its basic structure of this system determined by X-ray Rietveld analysis[14]. Here, information of local structures obtained from the ^{75}As -NMR/NQR spectra is given.

1. Results and Discussions

1.1. As NMR results for $\text{LaFeAsO}_{1-x}\text{F}_x$ and the nonexistence of the coherence peak

Figure 1 shows $\log[1/T_1/\{1/T_1(T_c)\}]-\log[T/T_c]$ curves obtained for As nuclei of $\text{LaFeAsO}_{1-x}\text{F}_x$ samples with various x values [4, 5, 7]. From the studies, we have found the following. (i) The coherence peak does not exist. (ii) A relation $1/T_1 \sim T^p$ can describe the curve well in the wide T region, $\sim 0.3 < T/T_c < 1.0$. The p value has the dome-shaped x dependence with a maximum value (~ 6) at the optimum $x \sim 0.11$. This x dependence is due to the fact that the spatial inhomogeneity of Δ within the samples becomes larger as x goes farther from the optimum x [5, 7, 8].

To study whether the nonexistence of CP is expected only for systems with sign reversal of Δ , we try to consider two effects on $1/T_1$: One arises from the quasi particle broadening, which is expected to be large in Fe pnictides, because they suffer from strong scatterings by the magnetic and/or orbital fluctuations (note that they are near the structural and antiferromagnetic instabilities). Another one is the rapid reduction of the spin susceptibility with growing Δ immediately below T_c . Here, learning the T -dependence of the energy broadening Γ of quasi-particles of $\text{YBa}_2\text{Cu}_3\text{O}_7$ [15], we express $\Gamma(T)$ form as

$$\Gamma(T) = \Gamma(T_c) \cdot \exp[a(T/T_c - 1)],$$

and choose the parameters $a=5.0$ and $\Gamma(T_c)=3k_B T_c$. This large $\Gamma(T_c)$ value is realistic, judging from the resistivity data. The value of $\Gamma(T)/\Gamma(T_c)$ below T_c is determined by the T dependence of the quasi particle number, and here, we adopted a realistic value $a=5$, comparing the rates of Δ , $|d\Delta/d(T/T_c)|$ of $\text{LaFeAsO}_{1-x}\text{F}_x$ ($x \sim 0.11$) and $\text{YBa}_2\text{Cu}_3\text{O}_7$ (For the latter, $a \sim 7.5$). Because we are just studying whether the coherence peak appears for Δ without sign reversal, it is enough to use these values describing the T dependence of Γ only near T_c . Using this Γ , we express the quasi particle density of state, $N_S(E)$ at $T \leq T_c$ as follows [16].

$$N_S(E) = N_N(E) \times \text{Re}[E - i\Gamma(T)] / [\{E - i\Gamma(T)\}^2 - \Delta^2],$$

with a constant Δ over the Fermi surfaces (E : the quasi particle energy). Then, an enhancement factor $[1 - \alpha_m(\mathbf{q})]^{-1}$ of the $\mathbf{q}$ dependent spin susceptibility χ_q is introduced to consider the

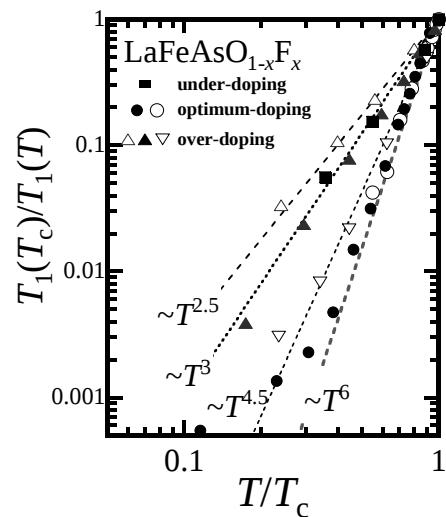


Figure 1. $(1/T_1)/(1/T_1(T_c))$ is plotted against $1/T$ for various x values of $\text{LaFeAsO}_{1-x}\text{F}_x$.

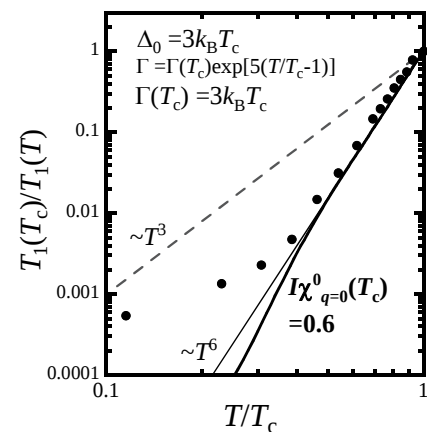


Figure 2. $1/T_1$ is calculated considering the T dependent energy broadening Γ of quasi particles and magnetic enhancement factor. Details are in the text.

Coulomb interaction of the quasi particles[17]. In antiferromagnetic (AF) samples, $\alpha_m(\mathbf{Q}_M)$ diverges at the Neel temperature T_N , where $\mathbf{Q}_M$ corresponds to the AF Bragg point. In superconducting samples, $\alpha_m(\mathbf{q})$ decreases rapidly with decreasing T below T_c , because it is proportional to the spin susceptibility of the quasi particles, the number of which also decreases rapidly. Even though $[1-\alpha_m(\mathbf{q})]^{-1}$ is rather large at $\mathbf{q}=\mathbf{Q}_M$, the value averaged over the $\mathbf{q}$ region of the large hyperfine coupling is not so large as can be found by the form factor consideration. We approximate this $[1-\alpha_m(\mathbf{q})]^{-1}$ by the $\mathbf{q}$ -averaged value $\langle 1/[1-\alpha_m(\mathbf{q})] \rangle$ to see its effect very crudely on $1/T_1$.

With the above considerations, we calculated $1/T_1(T)$, and show in Fig 2, with the logarithmic scales, the $(1/T_1(T))/(1/T_1(T_c))$ values against T/T_c for the S symmetry of Δ with the BCS type T dependence and for $\langle 1/[1-\alpha_m(\mathbf{q})] \rangle = 2.5$ at T_c . The observed data are also plotted for comparison. The calculation does not show the coherence peak, but shows the $\sim T^6$ dependence near T_c , indicating the possibility that the present type of calculations can reproduce the data of the observations. We do not think that it should reproduce the observed T dependence of $1/T_1$ in the wide T region, because of various reasons (which are not argued here). However, it indicates that the absence of the coherence peak cannot necessarily be connected with the existence of the sign reversal for systems which has strong fluctuations as Fe-based systems.

1.2. Ca-Fe-Pt-As system

As we have already reported elsewhere by the powder Rietveld analyses[14], two types of structure were identified for this Ca-Fe-Pt-As system, both of which have FeAs layers common to other pnictide systems. We used one of these systems with the type B (or HfCuSi₂ type) structure. The spectra were measured for samples ($T_c = 28$ K) with varying frequency in the temperature range from ~ 250 K down to T_c in the magnetic field of 5.8701 T. The spectra were also studied at 100 K with varying the direction of the magnetic field $\mathbf{H}$ with respect to the crystal axis.

Figure 3(a) shows the NQR spectra at 100 K which have two peaks at 11.355 and 11.93 MHz. They correspond to the nuclear electric quadrupole (eqQ) frequencies ν_Q at two crystallographically distinct As sites[14]. Figures 3(b) show the centerline of the NMR spectra at 100K for $\mathbf{H} \parallel \mathbf{c}$, where two components with distinct positions and widths were observed. The widths of both components are broader than those of the centerline of ^{75}As -NMR spectra observed for CaFe_2As_2 [18] and BaFe_2As_2 [19], indicating that Pt atoms are doped to Fe sites. Because the c -axis is the principal axis with the maximum ν_Q -value, the positions of the centerline are determined only by the Knight shift (not by eqQ effects). Therefore, we can find that there are two crystallographically distinct As sites in this system. It is consistent with the structure of ref. 14 with the alternating stacks of FeAs conducting layers and planar As layers: The sharp component at the higher- f position changing faster with T than that of the broad component is considered to correspond to the As-sites of FeAs layers, and those of planar As layers correspond to the As site in the planar layers, respectively.

Figure 4(a) shows the variation of the centerline of NMR spectra with the angle θ between $\mathbf{c}$ and $\mathbf{H}$, and the full width at half maximum (FWHM) of the line is plotted against θ in Fig. 4(b), where the local maximum of FWHM appears at $\theta \sim 20^\circ$ and $\sim 70^\circ$. (Note that the widths of both components become broader at those angles.) This θ dependence cannot be explained by the 2nd perturbation effects even for a larger distribution of ν_Q than that observed in NQR spectra, but can be explained by the distribution of angles between the principal axis with maximum ν_Q -value and c -axis as shown by solid curve in Fig. 4(b). This indicates that considerable large randomness exists at two As-sites,

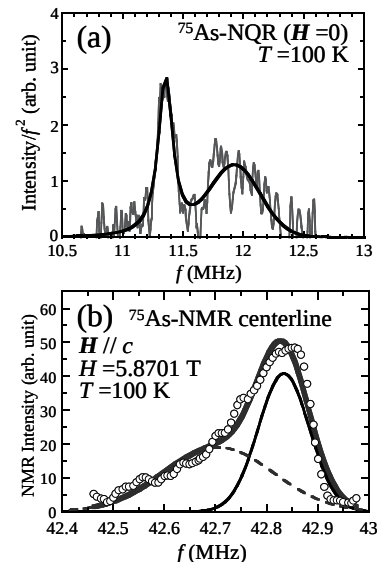


Figure 3. (a) ^{75}As -NQR spectra ($H=0$) and (b) centerline of ^{75}As -NMR spectra ($H \parallel c$) at 100 K. Two As sites can be seen.

which is consistent with the report that a large amount of Pt atoms are doped into the FeAs layers[14]. On this B type system, Ni *et al.* recently[20] carried out single crystal structure analyses, and reported its detailed superstructure with the distortion from our basic structure. They also found that the Pt atoms are heavily doped not only to the FeAs conducting layers, but also to planar As layer, which is also consistent with the broadening of both components of the centerline.

The considerable amount of the Pt-doping to the Fe-sites of the FeAs layers indicates that the possibility of the $S_{\pm}$ symmetry of the superconducting symmetry is not plausible, because the superconductivity should be strongly suppressed by the impurity scattering of the conduction electrons, if the order parameter has the sign reversal as in the case of the $S_{\pm}$ symmetry[5].

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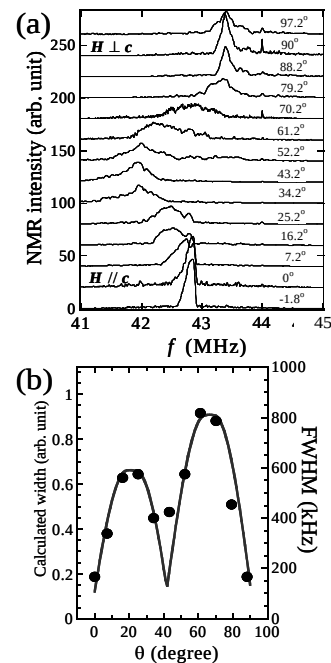


Figure 4. (a) ^{75}As -NMR centerlines for various $\mathbf{H}$ directions, the angles θ between $\mathbf{H}$ and $\mathbf{c}$ are attached to the lines. (b) FWHM's of the centerlines are shown