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Presence of Two Electronic States in $LaFeP_{1-x}As_xO_{0.95}F_{0.05}$

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1 Introduction

Superconductivity in iron-arsenide (Fe-As) compounds can be induced through carrier doping. Taking 1111 systems as an example, F doping suppresses the spin-density-wave (SDW) state and induces superconductivity with T_c as high as 55 K [1,2]. On the other hand, iron-phosphide (Fe-P) compounds are superconductors with relatively low T_c (<10 K) even without F doping [3-6]. Moreover, F doping in this kinds of compounds, LaFePO for instance, cannot change T_c significantly [7].

Revealed by experiments and theoretical calculations, the striking difference between Fe-As and Fe-P superconductors is due to the difference in their Fermi surface topologies [8-12]. In particular, the Fermi surface with d_{Z^2} orbital character appears at (π, π, π) in Fe-P compounds, while the Fe-As compounds have a cylindrical Fermi surface with the $d_{X^2-Y^2}$ orbital character [8]. Therefore, isovalent P/As substitution on 1111 systems is useful to understand the impact of Fermi surface topologies to superconductivity.

Previously we have investigated the physical properties of $R\mathrm{FeP}_{1-x}\mathrm{As}_x\mathrm{O}_{0.9}\mathrm{F}_{0.1}$ (R=La, Nd, Pr) [13]. For R = La, a maximum T_c ~ 28 K is observed and the temperature dependence of resistivity is mostly close to linearity at x = 0.6. Similar behaviors at x = 0.6 are also able to be observed in R = Nd and Pr which are different in lattice size. This suggests that these behaviours are driven by the electronic change due to P/As substitution, and that electronic change corresponds to the crossing of the d_{Z^2} band and the $d_{X^2-Y^2}$ band, i.e. a band crossover.

In this report we have studied the effect of P/As substitution on La1111 with lower F concentration (5%). Our results show that T_c is suppressed in the intermediate x-region between 0.5 and 0.7, giving two T_c peaks at around x = 0.4 and 0.8 respectively. The origin of these novel behaviors is also due to the band crossover via P/As substitution.

2 Experiment

The polycrystalline $LaFeP_{1-x}As_xO_{0.95}F_{0.05}$ with nominal x = 0 – 1 were synthesized by the conventional solid state reaction method. The precursors LaAs and LaP were first synthesized by reacting La powder and As grains/P powder in an evacuated quartz tube at 900 °C for 15 h and 700 °C for 10 h, respectively. LaAs, LaP, Fe_2O_3, Fe and LaF_3 were mixed with a stoichiometric ratio. The mixture was then grounded and pressed into a pellet. The pellet was annealed in an evacuated quartz tube at 1100 °C for 40 h. All processes were done in a glove box under argon and dry environment.

Superconducting transition was observed by measurements of resistivity conducted by a standard four-point-probe method. The determination of crystal structure was performed at room temperature by high resolution powder X-ray diffraction with the X-ray beam energy of 15 keV at BL-8A of Photo Factory (PF) in KEK, Japan. The lattice constants a, c and the pnictogen height h_{Pn} were calculated by a Rietveld refinement of the corresponding diffraction spectra using the software RIETAN-FP.

3 Results and Discussion

Temperature dependence of resistivity $\rho(T)$ of $LaFeP_{1-x}As_xO_{0.95}F_{0.05}$ is shown in Fig. 1. All samples exhibit the superconducting transition around 20 K, indicating the existence of bulk superconductivity. Moreover, $\rho(T)$ decreases with decreasing temperature without any anomalies, suggesting that all the samples are metallic and show no structural/magnetic phase transition.

Using the Rietveld refinement, all the Bragg peaks in the diffraction spectra can be well fitted within the tetragonal symmetry with the space group of $P4/nmm$ in all the samples. It indicates that the crystal structure is consistent with the previous report for the similar system La1111 [1].

The As-doping dependence of lattice constants a, c and h_{Pn} is shown in Figs. 2(a) and 2(b). All the parameters increase monotonically with x, indicating that the P/As-substituted samples have been successfully synthesized.

On the other hand, the superconducting properties of the samples show a different trend. The x dependence of T_c obtained from the resistivity measurements is shown in Fig. 2(c). Two peaks at x = 0.4 and 0.8, and a valley around x = 0.5 - 0.7 in the superconducting dome is able to be found, i.e. the value of T_c does not increase linearly with increasing x.

To further understand their behaviors, the temperature dependence of resistivity represented by the exponent n in $\rho(T) = \rho_0 + AT^n$ is obtained and the x dependence is plotted in Fig. 2(d). Here ρ_0 is the residual resistivity, and A is the slope of T^n. It is observed that the value of n is ~1 around x = 0.6, while it is ~2 at x ~ 0 and 1.0. It suggests that the samples around x = 0.6 are non-Fermi liquid while other samples are Fermi liquid. Moreover, this behavior is

similar to the results found in our previous study for $LaFeP_{1-x}As_xO_{0.9}F_{0.1}$ [13], suggesting that the band crossover may also happen around x = 0.6 in the current system.

Another clue can be seen in the plot of T_c against h_{Pn} for iron-based superconductors, as shown in Fig. 3 [14-17]. Previously Mizuguchi *et al.* [14] and Okabe *et al.* [15] have established this plot that shows a T_c peak at h_{Pn} of about 1.4 Å. The theoretical calculation has also supported that the value of h_{Pn} is one of the parameters to control the structure of the Fermi surface, and hence the gap symmetry and T_c in 1111 systems [8]. For $LaFeP_{1-x}As_xO_{0.9}F_{0.1}$ (the blue dots), the general trend is not followed at x = 0.6 [13]. This opposite trend suggests some abnormal behaviors in superconductivity cannot be characterized only by h_{Pn}, but also other factors, namely the band crossover. For $LaFeP_{1-x}As_xO_{0.95}F_{0.05}$ (the red dots), a similar behavior can be observed, in which T_c decreases with increasing h_{Pn} from x = 0.4 to 0.7. It again suggests that the similar band crossing observed in $LaFeP_{1-x}As_xO_{0.9}F_{0.1}$ is able to be found in $LaFeP_{1-x}As_xO_{0.95}F_{0.05}$.

Following the discussions in our previous study for $LaFeP_{1-x}As_xO_{0.9}F_{0.1}$ [13], these 2 peaks in $LaFeP_{1-x}As_xO_{0.95}F_{0.05}$ may represent two different electronic states based on the two Fermi surfaces, and they merge around x = 0.5 – 0.7. Upon P/As substitution, the crossover of the d_{Z^2} band and the $d_{X^2-Y^2}$ band occurs, and some novel properties are expected due to the change of the Fermi surface topologies. Since the minimum of T_c is located around x = 0.6, the band crossover probably occurs around x = 0.6 which is similar to the case of $RFeP_{1-x}As_xO_{0.9}F_{0.1}$ [13]. The origin of the T_c suppression induced by the crossover may be the anomalies in Fermi surface nesting condition or charge carrier concentration, but further investigation is necessary to confirm this idea.

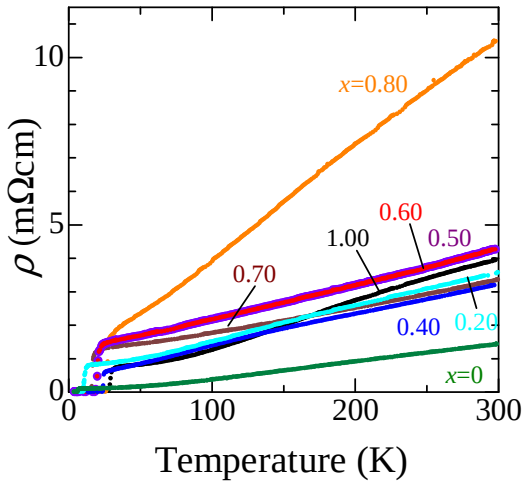

Fig. 1: Temperature dependence of resistivity of $LaFeP_{1-x}As_xO_{0.95}F_{0.05}$.

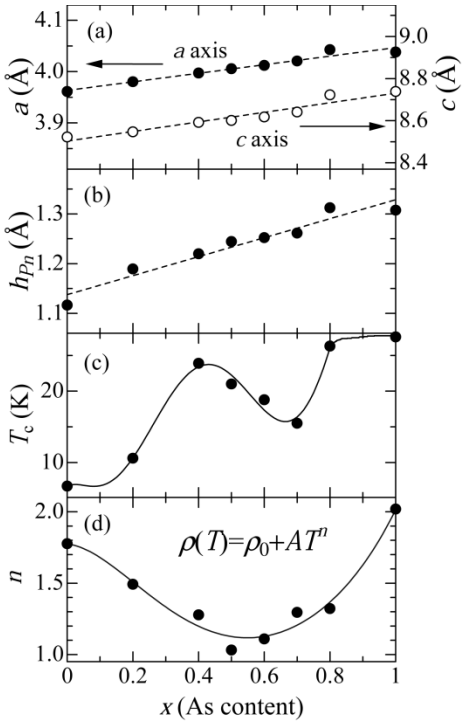

Fig. 2 The x dependence of (a) lattice constants a and c, (b) pnictogen height h_{Pn}, (c) critical temperature T_c, and (d) exponent n obtained from the temperature dependence of resistivity of $LaFeP_{1-x}As_xO_{0.95}F_{0.05}$.

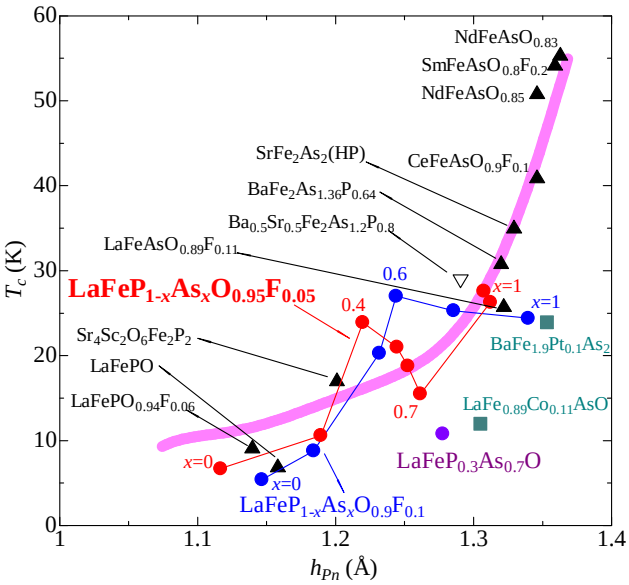

Fig. 3 The plot of T_c against h_{Pn} adapted from Mizuguchi *et al.* [14] and Okabe *et al.* [15]. The pink curve expresses the general trend for iron-based superconductors, which is constructed by Mizuguchi *et al.* The blue dots and red dots represent the data from $LaFeP_{1-x}As_xO_{0.9}F_{0.1}$ and $LaFeP_{1-x}As_xO_{0.95}F_{0.05}$, respectively. The value of x increases from 0 to 1 when the curves go from left to right.

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