

PCP5-1

Superconductivity in Uncollapsed Tetragonal LaFe_2As_2

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We report synthesis, crystal structure and superconductivity in ThCr_2Si_2 -type LaFe_2As_2 (La122). La122 was synthesized at 960°C for 1.5 h under a pressure of 3.4 GPa. An as-synthesized La122, which was *not* a superconductor, had a collapsed tetragonal structure with a short c -axis length of 11.0144(4) Å as observed in CaFe_2As_2 under pressure. The collapsed tetragonal transformed into an uncollapsed tetragonal by annealing the as-synthesized La122 at 500°C. The c -axis length remarkably extended to 11.7317(4) Å and superconductivity emerged at 12.1 K in the uncollapsed tetragonal La122. Ab-initio electronic structure calculations showed that a cylindrical hole-like Fermi-surface around the Γ point that plays an important role for an s_{\pm} wave pairing in iron-based superconductors was missing in the uncollapsed tetragonal La122 due to heavily electron-doping. Superconductivity in La122 may be closely related to that induced in CaFe_2As_2 under pressure.

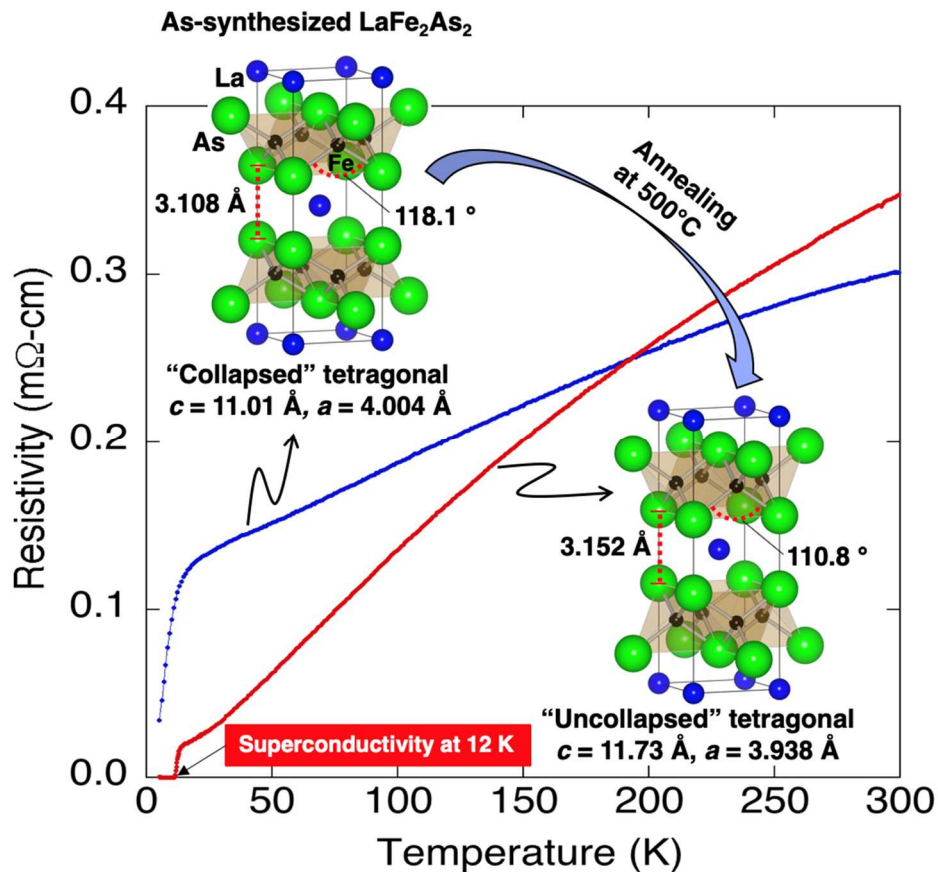


Figure 1 Temperature dependence of resistivity and crystal structures for as-synthesized and annealed LaFe_2As_2 .

Keywords: New superconductor, 122-type Iron-based superconductor, Collapsed tetragonal structure, Band structure calculation

PCP5-2

Electronic phase diagram of $\text{Sr}_2\text{V}_{1-x}\text{Sc}_x\text{FeAsO}_3$

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In iron-based superconductors, various electronic orders emerge in an iron layer due to intertwined electronic degrees of freedom. Iron-based superconductors with a perovskite-type thick blocking layer, e.g. $\text{Sr}_2\text{VFeAsO}_3$, offer various possibilities of chemical substitution into the blocking layer, which keeps the iron layer clean, and are suitable for a study to investigate the electronic state in the iron layer. $\text{Sr}_2\text{VFeAsO}_3$ shows superconductivity, while non-superconducting isostructural counterpart $\text{Sr}_2\text{ScFeAsO}_3$ exhibits antiferromagnetic ordering [1]. In this work, we synthesized polycrystalline $\text{Sr}_2\text{V}_{1-x}\text{Sc}_x\text{FeAsO}_3$ and studied how the electronic state evolves on going from $\text{Sr}_2\text{VFeAsO}_3$ to $\text{Sr}_2\text{ScFeAsO}_3$. With increasing Sc content x , a superconducting transition temperature systematically decreases. We revealed that the antiferromagnetic phase shows up for $x > 0.45$ adjacent to the superconducting phase. $\text{Sr}_2\text{VFeAsO}_3$ shows not only superconductivity but also an enigmatic electronic order at $T_0 \sim 150$ K. The phase transition at T_0 is present up to $x = 0.17$ and disappears with further Sc substitution. The suppression of the transition is slower than the case for Cr substitution [2]. In light of a proposed scenario that the transition at T_0 arises from frustration between stripe-type and Neel-type antiferromagnetic fluctuations of Fe and V spins, respectively [3], the frustration is lifted by non-magnetic Sc substitution at V sites, giving rise to the suppression of the transition.

[1] J. Munevar *et al.*, Phys. Rev. B **84**, 024527 (2011).

[2] T. Wakimura *et al.*, Supercond. Sci. Technol. **32**, 064003 (2019).

[3] J. M. Ok *et al.*, Nat. Commun. **8**, 2167 (2017).

Keywords: Iron-based superconductors, $\text{Sr}_2\text{VFeAsO}_3$, Chemical substitution

PCP5-3

Study of μ SR in Iron-Based Superconductor $\text{LaFeAs}_{1-x}\text{P}_x\text{O}_{0.9}\text{F}_{0.1}$

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In the iron-based superconductors $\text{LaFeAs}_{1-x}\text{P}_x\text{O}_{1-y}\text{F}_y$, the electron doping level and the local crystal structure can be controlled by the F substitution for O and P substitution for As. With these chemical substitutions, Fermi surface (FS) topology changes giving three different superconducting (SC) phases [1]. For example, at $y=0.1$, the As-rich compounds are in the first superconducting phase (SC1), while the P-rich compounds are in the second superconducting phase (SC2) [2]. The theoretical study by Kuroki and coworkers has indicated that the different nesting in LaFeAsO-type and LaFePO-type FSs induces the different SC gap symmetries, i.e., full and nodal gaps [3].

In the present work, we have investigated the difference between SC gap symmetry in SC1 and SC2 using μ SR measurement in $\text{LaFeAs}_{1-x}\text{P}_x\text{O}_{0.9}\text{F}_{0.1}$ ($x=0.0\sim 0.8$). The μ SR measurement were performed at TRIUMF in Canada and Research Center for Nuclear Physics (RCNP), Osaka University in Japan using a He gas-flow cryostat in a magnetic field of 250G. At $x=0$, the temperature (T) dependence of the muon spin relaxation rate σ shows a rapid increase with decreasing T below T_c and a saturation at low temperatures, indicating the s-wave behavior. In contrast, $\text{LaFeAs}_{1-y}\text{P}_y\text{O}_{0.9}\text{F}_{0.1}$ ($y=0.2\sim 0.8$) show the slightly different T dependence of the relaxation rate σ . In these P doping compounds, the T dependence of the relaxation rate σ does not show a clear saturation at low temperatures and cannot be fitted by the simple s-wave model. These results suggest that the P-doped compounds have several SC gaps with different gap sizes or a nodal SC gap, and the SC gap symmetries in the SC1 and SC2 phases may be different.

[1] S. Miyasaka *et al.*, Phys. Rev. B **95**, 214515 (2017).

[2] K. T. Lai *et al.*, Phys. Rev. B **90**, 064504 (2014).

[3] K. Kuroki *et al.*, Phys. Rev. B **79**, 224511 (2009).

Keywords: Iron-based superconductors, μ SR, superconducting gap

PCP5-4

Synthesis of the Mother Phase of the Iron-Based Superconductor, SmFeAsO via Low-Temperature Heat Treatment

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Low-temperature heat treatment of the iron-based superconductor^{1,2} is effective for fabrication of the iron-based superconducting wires and tapes with high transport critical current density. To determine the lowest temperature for the formation of a crystallographic phase of SmFeAsO, we demonstrate the evolution of the SmFeAsO during a solid-state reaction in a mixture of SmAs, Fe₂As, FeAs, and Sm₂O₃ heated to heat-treatment temperatures from 580°C to 950°C. X-ray diffraction (XRD) measurements indicated that a significant increasing of the SmFeAsO phase appears at heat-treatment temperatures not lower than 620°C. Scanning electron microscopy (SEM) with energy-dispersive X-ray spectroscopy (EDX) analysis showed a compound uniformly composed of samarium, iron, arsenic, and oxygen (Sm-Fe-As-O) having surface areas on the order of 10 μm² surrounded by grains of SmAs, Fe₂As, FeAs, and Sm₂O₃ in a sample heated to 580°C. This work therefore shows the SmFeAsO phase grows at 620°C and suggested that the SmFeAsO phase emerge at 580°C.

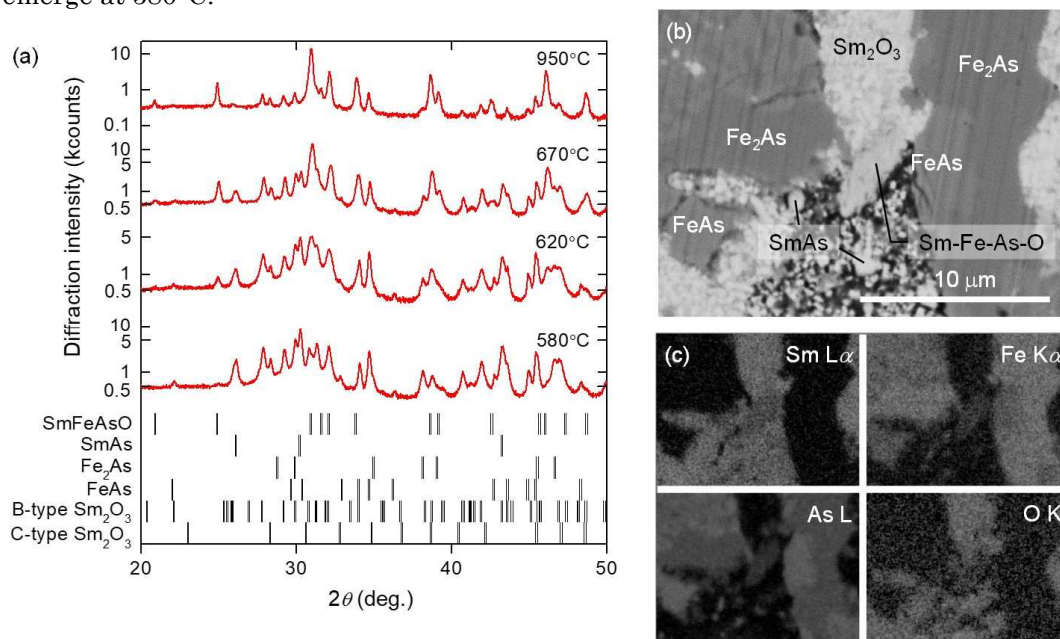


Fig. (a) Heat-treatment temperature dependence of X-ray diffraction (XRD) patterns at room temperature of the pulverized samples heated from SmAs, Fe₂As, FeAs, and Sm₂O₃ as starting materials. The vertical bars at the bottom represent diffractions due to SmFeAsO, SmAs, Fe₂As, FeAs, B-type Sm₂O₃, and C-type Sm₂O₃ from above. Heat-treatment temperatures are denoted near the patterns. (b) Back-scattered electron (BSE) scanning electron microscope (SEM) image and (c) energy-dispersive X-ray spectroscopy (EDX) elemental mapping of a polished sample heated to 580°C from SmAs, Fe₂As, FeAs, and Sm₂O₃ as starting materials.

[1] Y. Kamihara *et al.*, *J. Am. Chem. Soc.* **130**, 3296 (2008).

[2] Z.-A. Ren *et al.*, *Chin. Phys. Lett.* **25**, 2215 (2008).

Keywords: Iron-Based Superconductor, Solid-State Reaction, Low-Temperature Heat Treatment, Crystallographic phase

Fabrication of superconducting NdFeAs(O,H) epitaxial thin films

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$LnFeAs(O,F)$ (Ln : lanthanide) exhibits the highest superconducting transition temperature (T_c) up to 58 K among the Fe-based superconductors. However, the amount of F that can be substituted for O is limited to about 20% and it is difficult to investigate the physical properties in the overdoped region. On the other hand, Hanna *et al.* reported that the substitution limit can be increased to about 80% by changing the substituting elements from F to H[1]. Furthermore, SmFeAs(O,H) epitaxial thin films on MgO (001) substrates were grown recently using a topotactic reaction $SmFeAsO + (x/2)CaH_2 \rightarrow SmFeAs(O_{1-x}H_x) + (x/2)CaO$ [2]. It is interesting whether $LnFeAs(O,H)$ thin films for other Ln can be realized. Here, we report on the fabrication of NdFeAs(O,H) thin films using the same H doping method[2], and their structural and electro-magnetic properties.

Parent NdFeAsO thin films having a thickness of 20 - 30 nm were grown on MgO (001) substrates by molecular beam epitaxy[3]. The NdFeAsO film and CaH₂ powder were sealed in an evacuated quartz tube. The whole arrangement was then annealed under various conditions. Figure 1 (a) and (b) show the results of X-ray diffraction (XRD) measurement and the temperature dependence of resistance for one of the NdFeAs(O,H) films. For comparison, the data of an as-grown film are also shown. From the XRD measurements, no impurities were observed both for as-grown and annealed films. The 00 l peaks shifted to higher angles. The c -axis length changed from 8.587 Å to 8.466 Å. These results suggest that a phase-pure NdFeAs(O,H) film was obtained. The resistance measurement showed an onset T_c of 48 K and zero resistance at 45 K, respectively. The magnetization measurements exhibited a self-field critical current density of over 8 MA/cm² at 4 K, which is roughly comparable to our NdFeAs(O,F) films.

[1] T. Hanna *et al.*, *Phys. Rev. B* **84**, 024521 (2011). [2] J. Matsumoto *et al.*, arXiv:1903.11819 (2019). [3] T. Kawaguchi *et al.*, *Appl. Phys. Express* **4**, 083102 (2011).

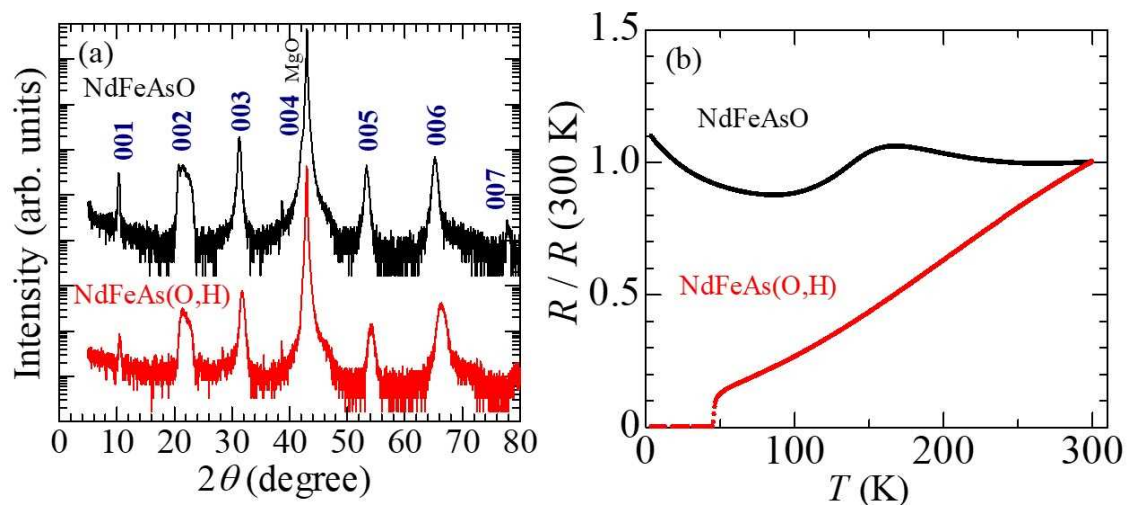


Fig.1. (a) XRD patterns and (b) the temperature dependence of resistance of non-doped and doped NdFeAs(O,H) thin films.

Keywords: oxypnictides, hydrogen doping, epitaxial thin films, topotactic reaction

PCP5-6

New strategies in PLD growth of iron-oxypnictides

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Pulsed laser deposition (PLD) in thin film growth of iron oxypnictides (ZrCuSiAs-type structure) faces several difficulties. Recently, further advances were made in the *in-situ* deposition of fluorine-doped oxypnictide films using fluorine diffusion from the substrate [1,2] or in hydrogen-doping based on an *ex-situ* diffusion process and a topotactic reaction [3]. Here we present a new strategy in the deposition of iron oxypnictides based on an iron pnictide template (BaFe₂As₂). This approach does not only allow a reduction of lattice mismatch between film and substrate but also offers a compatible chemical bonding environment at the interface resulting in a common FeAs-layer. For the purpose of investigating how superconductivity is affected by this specific template approach we turned to Co-doped iron oxypnictides (SmOFe_{1-x}Co_xAs and LaOFe_{1-x}Co_xAs). Our analysis combines structural and analytic investigations using XRD, TEM, electrical transport measurements and AES depth profiling. We will finally discuss the role of diffusion processes in iron oxypnictides in comparison with previous results on F-doped thin films with a diffusion-gradient hybrid structure [4]. The results demonstrate how diffusion affects the superconducting state of individual iron-pnictide layers.

References

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- [4] S. Haindl, E. Kampert, M. Sasase, H. Hiramatsu, H. Hosono, *Supercond. Sci. Technol.* **32**, 044003 (2019)

Keywords: iron pnictides, thin films, pulsed laser deposition

PCP5-7

AC, DC and magnetic relaxation studies of cuprate and pnictide superconducting single crystals exhibiting a second magnetization peak

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We investigated the AC magnetic response of several $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and 122-type pnictide superconducting single crystals exhibiting a pronounced DC Second Magnetization Peak (SMP). It was found that in the case of small demagnetization effects (LSCO samples) the AC magnetic signal across the SMP remains in the linear regime, with no detectable distortions in the SMP range, which indicates reduced values of the Campbell penetration depth.

The nonlinear AC Bean regime far below the Irreversibility Line has been observed in plate-like 122-type pnictide specimens in perpendicular magnetic fields with strong demagnetization effects. The origin of SMP in superconducting single crystals with fourfold symmetric inter-vortex interactions (such as $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and the 122-type iron pnictides) has been directly related to the structural rhomb-to-square vortex-phase transition (ST). At the same time, for various superconducting systems, the SMP was attributed to a pinning-induced disordering of the quasi-ordered vortex solid, the proliferation of dislocations in the vortex system leading to a better accommodation of vortices to the pinning centres.

We discuss the relevance of these two models for the SMP in fourfold symmetric superconductors, by investigating the isothermal DC magnetic hysteresis curves $m(H)$, the DC magnetization relaxation, and the AC magnetic response of overdoped $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ single crystal, where both the SMP and the ST are expected to be present. It was found that the ST leads to a “shoulder” on the $m(H)$ curves, affecting the onset of the SMP. The enhancement of the $m(H)$ shoulder with decreasing temperature leads to the intersection of magnetic hysteresis curves, and, consequently, to a peak in the temperature variation of the critical current density. However, in AC magnetic measurements, when the vortex system is dynamically ordered in the ST range, there is no sign for such a peak at the structural transition temperature. This indicates that the $m(H)$ shoulder is generated by a precipitous pinning-induced proliferation of dislocations in the vortex system at the ST, where the “squash” vortex-lattice elastic modulus softens.

Keywords: single crystals, pnictides, cuprates, Second Magnetization Peak