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Citation: AIP Advances 6, 075104 (2016); doi: 10.1063/1.4958873
View online: http://dx.doi.org/10.1063/1.4958873
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Pressure-induced shift of $T_c$ and structural transition in “122” type pnictide superconductor $\text{Ca}_{0.34}\text{Na}_{0.66}\text{Fe}_2\text{As}_2$

Sijia Zhang,¹,a Kan Zhao,¹ Xiaohui Yu,¹,² Jinhong Zhu,³ Qingqing Liu,¹ Xiancheng Wang,¹ Shaomin Feng,¹ Zhiqiang Chen,⁴ Yusheng Zhao,² and Changqing Jin¹,a

¹Institute of Physics, Chinese Academy of Sciences, Beijing100190, China
²Los Alamos Neutron Science Center (LANSCE), Los Alamos National Laboratory, Los Alamos, New Mexico 87545, United States
³High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, United States
⁴National Synchrotron Light Source, Brookhaven National Laboratory, Upton, New York 11973, United States

(Received 26 May 2016; accepted 1 July 2016; published online 11 July 2016)

The effect of pressure on superconductivity of “122” type $\text{Ca}_{1-x}\text{Na}_x\text{Fe}_2\text{As}_2$ ($x=0.66$) single crystal is investigated through the temperature dependence of resistance measurement. Optimal Na doped ($\text{Ca}_{0.34}\text{Na}_{0.66})\text{Fe}_2\text{As}_2$ shows a superconducting transition with $T_c \sim 33$ K at ambient pressure. With application of pressure, $T_c$ decreases nearly linearly with $dT_c/dP \sim -1.7$K/GPa at pressures lower than 2 GPa, and disappears gradually at higher pressure. The disappearance of superconductivity is also accompanied with the recovery of normal Fermi liquid behaviors of the normal-state transport properties. Moreover, ($\text{Ca}_{0.34}\text{Na}_{0.66})\text{Fe}_2\text{As}_2$ exhibits a tetragonal (T) to collapsed-tetragonal (cT) transition at about 3 GPa. The evolution of non-Fermi liquid behaviors and superconductivity under pressure are both related to the interband fluctuations. © 2016 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/). [http://dx.doi.org/10.1063/1.4958873]

INTRODUCTION

The superconductivity of LaO$_{1-x}$F$_x$FeAs with $T_c \sim 26$K has attracted much attention in high temperature superconductor research field as the transition temperature ($T_c$) is only second to the high $T_c$ cuprates, and many pnictide superconductors were investigated from then on.²–⁹ Similar to “1111” parent compounds, CaFe$_2$As$_2$ with tetragonal ThCr$_2$Si$_2$-type structure exhibits a spin-density wave (SDW) transition at about 165K, accompanied with a structural phase transition at the Ca site subsequently. A higher $T_c \sim 33$ K in ($\text{Ca}_{0.32}\text{Na}_{0.68})\text{Fe}_2\text{As}_2$ has also been reported,¹⁸ with the two-thirds Na doping at the Ca site, so-called optimal doping. Furthermore, the pressure-tuned superconductivity has been reported in some “1111”, “122”, “111”, or “11”-type pnictide compounds as well.¹⁹–²⁷ For some compounds, the superconductivity can be initiated by pressure and the $T_c$ can be pushed to a maximum with initial compression, whereas for some other compounds the $T_c$ is suppressed by application of pressure monotonously. It has been explained that the $T_c$ of pnictide superconductors is closely related to the

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¹Author to whom correspondence should be addressed. Electronic mail: sjzhang@iphy.ac.cn, jin@iphy.ac.cn
The geometric change of the FeAs₄ tetrahedron as well as the anion height from Fe layer,²⁸,²⁹ which is also experimentally confirmed.³⁰,³¹ CaFe₂As₂ is somehow different from BaFe₂As₂ or SrFe₂As₂ as due to its reduced unit cell volume and c lattice parameter, which is very close to collapsed tetragonal (cT) phase. So it is very sensitive to external pressure and chemical pressure (doping). A pressure-induced tetragonal-to-collapsed tetragonal structure phase transition was observed in CaFe₂As₂ above 0.35 GPa at 50 K.³² We focus on (Ca₀.₃₄Na₀.₆₆)Fe₂As₂ in this work since it shows the highest Tc of ~ 33 K for (Ca₁₋ₓNaₓ)Fe₂As₂. The high-pressure resistance measurements and the high-pressure X-ray diffraction experiments for optimal doped (Ca₀.₃₄Na₀.₆₆)Fe₂As₂ are performed. We mainly discussed the influence of T to cT phase transition on the superconductivity. The resistance changes its low-energy behavior from \( \rho \propto T^{1.3} \) in the T phase to \( \rho \propto T^2 \) in the cT phase, with the disappearance of superconductivity. The interplay of superconductivity and collapsed tetragonal phase suggests the essential role of magnetic fluctuations in the emergence of superconductivity.

EXPERIMENTAL DETAILS

The (Ca₀.₃₄Na₀.₆₆)Fe₂As₂ single crystals were synthesized using the solid-state reaction method. The detailed conditions and process of synthesis were described in Refs. 16 and 33.

The pressure-induced evolution of Tc in (Ca₀.₃₄Na₀.₆₆)Fe₂As₂ single crystal was investigated by four-probe electrical resistance measurement methods at variant pressures. The experiments were performed using both piston-cylinder-type pressure cell with liquid transmitting medium silicone oil and diamond anvil cell (DAC) with solid transmitting medium hexagonal boron nitride (h-BN). In piston-cylinder-type pressure cell, the silicone oil was used as pressure-transmitting medium to measure the temperature dependence of resistance under different hydrostatic pressures. The size of the sample was about 1.5 x 0.9 x 0.05 mm³. All the pressure values quoted in this paper were measured at room temperature. For DAC experiment, pressure was generated by a pair of diamonds with 500-µm-diameter culet. The stainless steel gasket was pre indented from 250 µm to ~40 µm thickness with a 250-µm hole in the center that serves as the sample chamber. The sample size was about 100 µm × 100 µm × 30 µm. The pressure was determined by ruby fluorescence method at room temperature before and after each cooling down. The DAC experiments were performed twice with two different samples.

The X-ray diffraction experiments at high pressure with synchrotron radiation were done at the National Light Synchrotron Source (NSLS) of the Brookhaven National Laboratory with a wavelength 0.407 Å using a symmetric Mao Bell diamond anvil cell at room temperature. The crystal structures were refined using GSAS package.³⁴

![FIG. 1. The X-ray diffraction of (Ca₀.₃₄Na₀.₆₆)Fe₂As₂ single crystal. Inset: Temperature dependent magnetization of (Ca₀.₃₄Na₀.₆₆)Fe₂As₂ superconductors at ZFC conditions with H=300e.](image-url)
RESULTS AND DISCUSSION

The (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$ single crystals used in the high pressure experiments has a single-phase nature. Fig. 1 shows the X-ray diffraction pattern of (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$ single crystal with (00l) peaks. The magnetization curve shows sharp superconducting transition around 33K with full shielding fraction, which indicates the good quality of the sample. Fig. 2(a) shows the in-plane resistance $R_{ab}$ of (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$ as a function of temperature at different pressures up to 2.4 GPa using piston-cylinder-type pressure cell. Above 2 GPa, the width of superconducting transition increases apparently, from 0.5 K at pressures lower than 2 GPa to 3 K at 2.4 GPa. Because of the limitation of pressure in piston-cylinder-type pressure cell, we also perform the high-pressure resistance experiments using DAC cell, the results of two times are shown in Fig. 3. The width of superconducting transition increases rapidly with increasing pressure so that the zero-resistance disappears above 2 GPa, and the superconducting transition disappears completely at higher pressures. The values of $T_c$ at variant pressures are determined from the intersection of two extrapolated lines, which extract from the experimental curve before and after transition as shown in Fig. 2(b). The $T_c$–pressure phase diagram of (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$ from piston-cylinder-type pressure cell is

![Diagram](image-url)
FIG. 3. (a) The temperature dependence of in-plane resistance $R_{ab}$ for (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$ single crystals at variant pressures up to 3.7 GPa using DAC cell; (b) The second experiment using DAC cell at variant pressures up to 6.9 GPa.

shown in Fig. 4. It is noteworthy that $T_c$ decreases linearly as the pressure increases with a slope $dT_c/dP = -1.7$ K/GPa. The $T_c$ evolution behavior with pressure is closely related to the change of strong Fermi surface nesting between hole and electron sheets through tuning the As-Fe-As bond angles and the anion height from Fe layer directly by pressure. So pressure probably makes the structure distort away from optimal position so that $T_c$ decreases with increasing pressure in (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$.

To investigate the normal-state transport properties of (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$, the formula $R(T) = R_0 + AT^\alpha$ is used for fitting the low-temperature part of R-T curve beyond transition temperature, the result is shown in Fig. 5. It exhibits an approximate $T$-linear dependence in a wide temperature range ($T_c < T < 130$ K) at 0.2 GPa, which suggests a strong similarity to the non-Fermi-liquid (non-FL) behaviors governed by quantum fluctuations in strongly correlated electron systems. Similar anomalous $T$-linear behaviors that deviate from the standard Fermi-liquid (FL) properties have been reported in several Fe-pnictides. With increasing pressure, $\alpha$ increases and the FL behavior recovers gradually. The width of superconducting transition of (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$ also increases rapidly with the recovery of FL behavior. The Fermi surface structure with interband nesting plays an important role for superconductivity in Fe-pnictides. Thus there must be a large
FIG. 4. The $T_c - P$ phase diagram of $(\text{Ca}_{0.34}\text{Na}_{0.66})\text{Fe}_2\text{As}_2$ obtained from resistance measurements. Experimental data are the points with error bar. The pattern of As-Fe-As bond angles and anion height from Fe layer is also given, the blue spheres are As atoms (all around), and the yellow sphere is Fe atom (middle).

change of Fermi surface nesting between the hole and electron sheets induced by pressure, which resulting the non-FL to FL transition. For $(\text{Ca}_{0.34}\text{Na}_{0.66})\text{Fe}_2\text{As}_2$, the width of superconducting transition of R-T curve increases and zero-resistance disappears above 2 GPa. The phenomena indicate that the sample is no longer a single phase. To further investigate the evolution of structure of $(\text{Ca}_{0.34}\text{Na}_{0.66})\text{Fe}_2\text{As}_2$ under high pressure, we perform the high pressure X-ray diffraction experiments. Fig. 6(a) shows the synchrotron X-ray diffraction pattern for a wide angle range from ambient pressure up to 5.1 GPa at room temperature. Each peak is labeled with the corresponding (hkl). The GSAS program software package is used to obtain the lattice parameters at each pressure, which is listed in Fig. 6(b). With increasing pressure, the $c$ axis shrinks and $a$ axis slightly expands, between 2.3 GPa and 3.1 GPa, there is a rapid reduction as large as $\sim$6% of the $c$ axis whereas the $a$ axis expands by $\sim$1%, indicating the T to cT phase transition, which has been reported in the parent CaFe$_2$As$_2$ under pressure. With further increasing pressure, both $a$ axis and $c$ axis smoothly decrease. Because of the destruction of interband nesting in cT phase, the lack of magnetic fluctuations could be responsible for the recovery of FL behaviors and the absence of superconductivity.

FIG. 5. The low-temperature part of R-T curves ($T_c < T < 130$ K) can be fitted by the formula as shown in the figure, which exhibits a change from approximately $T$-linear to $T$-square dependence of resistance.
FIG. 6. (a) The synchrotron X-ray diffraction pattern for a wide angle range from ambient pressure up to 5.1 GPa at room temperature. Each peak is labeled with the corresponding (hkl) at 0 GPa and 3.1 GPa respectively; (b) Pressure dependence of crystal parameters $a$, $c$ and volume, which shows a T to cT phase transition.

FIG. 7. The pressure-temperature phase diagram of (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$. 
Similar with (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$ in cT phase, both the absence of superconductivity and the recovery of FL behaviors have also been observed in cT phase of CaFe$_2$As$_2$ or doped Ca122 Fe pnictides.  

In summary, we have shown that the $T_c$ of (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$ decreases nearly linearly with a slope $dT_c/dP$ $\sim$ $-1.7$ K/GPa with increasing pressure. Anomalous non-FL behaviors of R-T curves are also observed at lower pressures in (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$, whereas the recovery of FL transport properties corresponds to the disappearance of superconductivity. Meanwhile, (Ca$_{0.34}$Na$_{0.66}$)Fe$_2$As$_2$ exhibits a tetragonal (T) to collapsed-tetragonal (cT) transition at about 3GPa according to high pressure synchrotron X-ray diffraction experiments. The pressure–temperature phase diagram is shown in Fig. 7. The results strongly suggest that the superconductivity and the observed non-FL transport properties are both closely related to the interband-associated strong spin and orbital fluctuations in Fe pnictides.

ACKNOWLEDGMENTS

This work is supported by NSF and MOST of China through research projects.