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Pressure effects on iron-based superconductor $CaFe_{0.88}Co_{0.12}AsF$

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Abstract

Systematic measurements of electrical resistivity and Hall coefficient under high pressure were performed on $CaFe_{0.88}Co_{0.12}AsF$ single crystal samples. The superconductivity is suppressed quickly by pressure and can not be detected down to 2 K at above 12.7 GPa, while the magnitude of the Hall coefficient R_H shows a very weak pressure and temperature dependence. A comprehensive analysis considering the pressure dependence of T_c, R_H, residual resistivity ratio, and the Fermi-liquid term of the resistivity indicates that the electron correlation is an important factor in superconductivity of iron-based superconductors.

Keywords: superconductivity, pressure, phase diagram

(Some figures may appear in colour only in the online journal)

The key factor which determines the superconducting critical transition temperature T_c is a central issue in the field of unconventional superconducting materials and physics. In the iron-based superconductors (FeSCs), empirically a correlation between T_c and the bond angle/Pnictogen height was revealed and a regular tetrahedron configuration in the FeAs layer was found to be profitable to superconductivity [1]. This tendency has been interpreted from different aspects [2, 3, 4]. Based on the weak electron correlation picture, Fermi surface (FS) nesting was believed to be very crucial for the iron-based superconductivity [5, 6]. Later on, a unified phase diagram of FeSCs based on electron correlation strength was obtained from the systematic angle resolved photoemission spectroscopy (ARPES) studies, which challenged the weak correlation picture [7, 8]. Recently, a theoretical work considering various material including metal, Heavy Fermion, MgB_2, FeSCs and cuprates showed that the fluctuation of the orbital hybridization is crucial for T_c [9]. Typically multiple factors are associated with superconductivity and it is a great challenge to identify the most important one and reaching a solid conclusion.

Pressure plays a significant role in the field of superconductors. For example, the T_c of FeSe is enhanced to about 37 K while the T_c at ambient condition is 8 K [10]. Pressure can also induce superconductivity in the parent compound where superconductivity is absent [11–13], induce a second superconducting phase [14], and tune the system to a quantum critical point at zero temperature [15]. More importantly, pressure can provide a clean way to tune the ground state continuously without introducing disorders and dopants. This advantage may simplify the complicated systems and benefit the extraction of the key factors determining T_c.

Among different systems, the 1111 family holds the record of T_c of FeSCs [16, 17]. AEFeAsF (AE = Ca, Sr, Eu) is a new member of the 1111 family with the same crystal structure as LaFeAsO but with oxgen free [18–20]. Recently, fascinating features including nontrivial Dirac Fermions were revealed [21–25] due to the improvements in the size and quality of single crystal samples [26, 27]. In this paper, we tune a $CaFe_{0.88}Co_{0.12}AsF$ single crystal sample, which is superconducting with $T_c = 21$ K at ambient conditions, by applied pressure up to 17.2 GPa. We study systematically the evolution of the normal and superconducting states with increasing pressure. The superconducting transition temperature and the normal state resistivity of this sample are suppressed quickly by increasing pressure. In contrast, the Hall coefficient R_H and the residual resistivity ratio are found to remain unchanged with pressure. These results suggest that the electron correlation plays more important role than charge carrier concentration and Fermi surface structure on superconductivity.

High quality single crystal samples of $CaFe_{1-x}Co_xAsF$ were synthesized by CaAs self-flux method [26, 27]. Electrical resistivity measurements were performed using a Quantum Design Physical Property Measurements System (PPMS). The current is applied in the *ab* plane and the magnetic field is applied along the *c*-axis of the crystal. Pressure was applied at room temperature using diamond anvil cells (DAC) made of CuBe alloy (Easylab CryoDAC-PPMS), with the diamond anvil culet of 500 μm in diameter. The van der Pauw method was used to complete high-pressure electrical resistivity and Hall coefficient measurements simultaneously. Daphne oil 7373 was used as the pressure transmitting medium. Pressure was calibrated using the ruby fluorescence shift at room temperature.

Figure 1(a) shows the temperature dependent resistivity $\rho(T)$ curves for $CaFe_{0.88}Co_{0.12}AsF$ measured under different pressures up to 17.2 GPa. The inset to figure 1(a) shows the resistivity curve at ambient condition. Note that it is measured on a difference piece of sample from the one loaded in the DAC. The order of magnitudes of the resistivity is consistent with previous report on other 1111 systems [22, 28–30]. With increasing pressure, the resistivity ρ at 300 K decreases monotonically, similar to the previous report on polycrystal $CaFe_{1-x}Co_xAsF$ [28]. In the low temperature region, a superconducting transition can be observed, which is shifted to lower temperatures by the pressure. Such a superconducting transition is suppressed completely when the pressure is higher than 12.7 GPa.

Before entering the superconducting state, a resistivity minimum can be observed at T_{dip} followed by an upturn of the resistivity exhibiting a semiconductor-like behavior (see figure 1(b)). This is consistent with previous reports on other FeSCs in the underdoped region [18, 27, 28, 30–35]. The origin of the upturn behavior is unclear at present. Co substitution introduces scattering centers, local structural disorder, Kondo effect, and weak localization effect have been proposed to interpret this behavior [28, 30]. Notably, pressure tuning of the parent CaFeAsF compound also leads to the resistivity upturn at low temperature [13], which contradits the scattering and disorder scenario. We found that the upturn

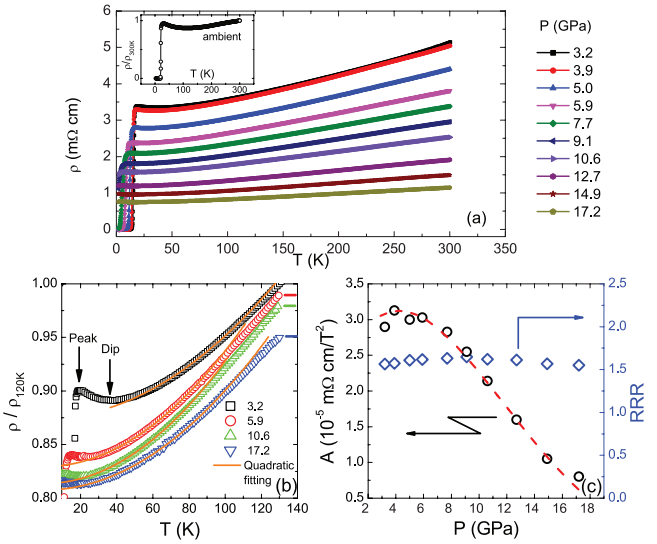

Figure 1. (a) Temperature dependence of resistivity ρ under different pressures. Inset shows the data at ambient condition which is measured on a difference piece of sample from the one loaded in the DAC. (b) The enlarged plot in the low temperature for the data at $P = 3.2$, 5.9, 10.6, and 17.2 GPa. For clarity, the data have been normalized by the value at 120 K and shifted downward. The yellow curves represent the results of a quadratic fitting based on the Landau Fermi liquid theory. (c) The pressure dependence of the fitting parameter *A* and residual resistivity ratio *RRR*.

behavior of our sample is very robust and survives even at the pressures as high as 17.2 GPa, where the superconductivity has been suppressed. This might suggest a superconductor to insulator transition.

We summarized the pressure dependence of T_c, T_{peak} and T_{dip} in figure 2. T_c is defined by 90% of the normal state resistivity ρ_n and it is suppressed quickly by increasing pressure, which is similar as the tendency of $T_c(P)$ in parent compound of CaFeAsF [13, 28]. The resistivity minimum decreases with increasing pressure until a critical pressure of 12.7 GPa, then it slightly increases and shows the tendency of saturation. Note that this critical pressure is corresponding to the point where superconductivity vanishes. The T_{peak} decreases monotonically with increasing P, and vanishes for P higher than 12.7 GPa.

We also measured the $\rho - T$ curves at low temperatures under different applied magnetic field H. Figure 3(a) shows the resistivity curves for $P = 3.9$ GPa, which represent the typical behaviors of our sample under pressure. With increasing H, the superconducting transition shifts to lower temperature. The temperature dependence of the upper critical field H_{c2} under different pressures are plotted in figure 3(b). Here, the superconducting transition temperature T_c is also defined as $90\%\rho_n$. Note that there is a clear upward curvature in $H_{c2}(T)$, suggesting the multiband nature of superconductivity, which is typical for FeSCs. This deviation from the Werthamer–Helfand–Hohenberge (WHH) theory which is based on the single-band model is probably a consequence of a nonspherical Fermi surface. As was shown by Hohenberg and Werthamer [36], the zero-temperature value of H_{c2} for samples with nonspherical Fermi surfaces, is always larger than $H_{c2}(0)$ determined by using the WHH formula proposed for a weak-coupling

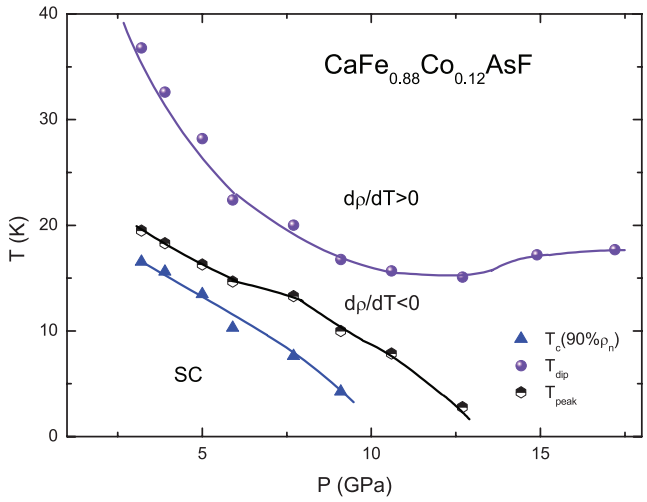

Figure 2. Temperature versus pressure ($T-P$) phase diagram of $CaFe_{0.88}Co_{0.12}AsF$. T_{dip} is the resistivity minimum which corresponds to the crossover temperature from metallic to semiconductor-like behavior. T_{peak} represents the temperature of the resistivity maximum before entering the superconducting state. The superconducting transition temperature T_c is determined by the criteria 90% of the normal state resistivity.

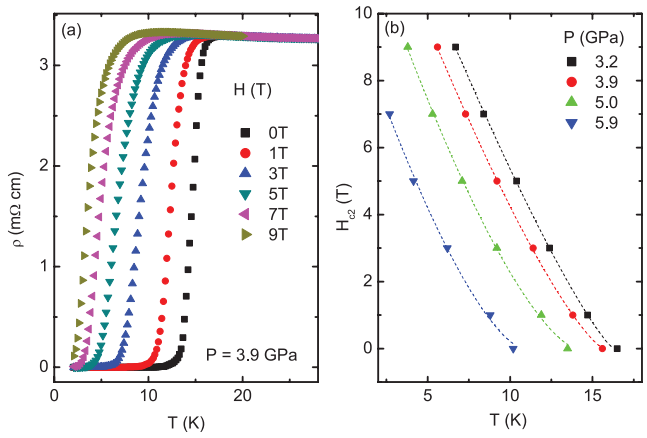

Figure 3. (a) Typical low-temperature-dependent resistivity curves with different fields parallel to the c axis at $P = 3.9$ GPa. (b) The temperature dependent upper critical field H_{c2} curves under four different pressures. The dashed lines are fitting curves by $H_{c2}(T) = H_{c2}(0)(1 - T/T_c)^{\alpha}$.

superconductor, i.e. $H_{c2}(0) = 0.693(-\mathrm{d}H_{c2}/\mathrm{d}T)_{|T=T_c}$. It is found that the data of $CaFe_{0.88}Co_{0.12}AsF$ can be fitted by the simple relationship of the form $H_{c2}(T) = H_{c2}(0)(1 - T/T_c)^{\alpha}$, which was used before [13, 37–39]. The fitting parameter H_{c2} can be considered as the upper limit for the upper critical field $H_{c2}(0)$ [36, 38, 39]. With increasing pressure, the value of $H_{c2}(0)$ is monotonically suppressed. $H_{c2}(0)$ is in the range of 17.1 T–10.6 T for P range 3.2–5.9 GPa. The corresponding α is from 1.22 to 1.48, comparable with similar iron-based superconductors [40].

Next, we study the Hall resistivity ρ_{xy} which is measured simultaneously with resistivity. Figure 4(a) plots H dependence of ρ_{xy} under different pressures. It is found that ρ_{xy} shows a linear relation with H and the slope of the curves remains almost unchanged with pressure. The obtained R_H is plotted

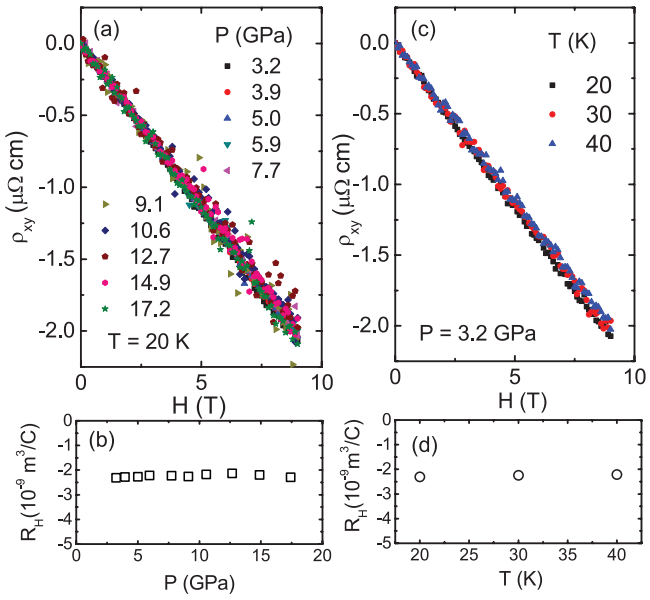

Figure 4. (a) Magnetic field dependence of Hall resistivity ρ_{xy} of 20 K at different pressures from 3.2 to 17.2 GPa. (b) Pressure dependence of Hall coefficient R_H at $T = 20$ K. (c) ρ_{xy} versus H at $T = 20$, 30 and 40 K under the pressure 3.2 GPa. (d) Temperature dependence of R_H for $P = 3.2$ GPa.

in figure 4(b), which shows a very weak pressure dependence. This means the charge carrier density n and the Fermi surfaces are not influenced by pressure. The magnitude of R_H is in the order of 10^{-9} m^3/C, similar to other FeSCs [40–43]. At $P = 3.2$ GPa, ρ_{xy} and R_H at different temperatures $T = 20$, 30 and 40 K are shown in figures 4(c) and (d). It is found that the change of ρ_{xy} and R_H with temperature is also rather weak.

We must emphasize that the pressure independent Hall coefficient R_H is very important, which simplifies the issue to check the influence factors on superconductivity (i.e. T_c). With the increase of pressure, the fact that R_H remains unchanged while T_c decreases indicates that the charge carrier density and even the shapes of Fermi surfaces are not important for the superconductivity. Obviously this fact challenges severely the Fermi surface nesting picture [5, 6], which is rather consistent with our recent results on the gap structure of this system [44]. We note that such a conclusion from our single material system also confirms the declaration of Feng's group from the measurements of ARPES on various FeSCs [7, 8]. Moreover, as we have noticed, resistivity in the normal state is also suppressed by pressure (see figure 1(a)). Based on the simple Drude model $\rho = m^*/nq^2\tau$ (m^* is the effective mass of electrons, q is charge of a electron, τ is the scattering relaxation time), the changes of ρ is only determined by the m^* and τ. Typically high pressure does not introduce disorders and other extra effects to the system, thus the relaxation time τ should not change a lot. Such an analysis is further supported by the pressure independent residual resistivity ratio (RRR) (as shown in figure 1(c)), which mainly reflects the ratio of τ between T-dependent term (electron–phonon scattering and electron–electron scattering) and T-independent term (scattering with impurities and disorders), because we can not imagine both of these two terms can change in lock-step with pressure.

The only remaining possibility is that the effective mass m^*, which is mainly affected by the electron–phonon interaction and electron correlation [45], is suppressed by the applied pressure. In order to clarify the crucial mechanism for this variation, we further checked the T-dependent resistivity data based on the Landau Fermi liquid theory (FL theory). According to FL theory, the low temperature resistivity data can be described by a T^2 term and the coefficient of this term is a measure of the strength of electron-electron correlation [46, 47, 48]. Typically the FL behavior is distinct in low temperature region, so we display the resistivity data in the low temperature under four different pressures in figure 1(b). We fitted the data with the formula $\rho = \rho_0 + AT^2$, where ρ_0 and A are the fitting parameters. The lower temperature limit for the fitting is several Kelvins above $T_{\rm dip}$. While the upper limit is determined by checking the derivative of the $\rho - T$ curve and the point where the $\mathrm{d}\rho/\mathrm{d}T$ curve departs from the linear behavior is selected. Within this temperature range, the data can be well described by FL theory, as shown by the yellow curves in figure 1(b). The coefficient of the quadratic term A under different pressures is summarized in figure 1(c). Importantly, a clear suppression of A by pressure can be seen. It is notable that the values of A have a same order of magnitude as other correlated electron systems [14, 48] and the absolute variation of A induced by pressure is more conspicuous in our case. So now we know that it is the suppression of electron correlation strength that accompanies the decrease and even disappearance of $T_{\rm c}$.

In summary, we performed pressure dependent transport measurements on $CaFe_{0.88}Co_{0.12}AsF$. It is found that this material is a very good prototype to distinguish the complicated influence factors on $T_{\rm c}$, because both the $R_{\rm H}$ and *RRR* are not affected by pressure. Meanwhile, $T_{\rm c}$ and the electron correlation strength are suppressed by pressure. A comprehensive analysis shows that the charge carrier density and Fermi surface structure are not important for the superconductivity of FeSCs, and the electron correlation is the most important influence factor on $T_{\rm c}$.

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