Electronic and lattice structure of CaFe$_{1-x}$Co$_x$AsF probed by x-ray absorption spectroscopy

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Abstract

The local lattice and electronic structures of CaFe$_{1-x}$Co$_x$AsF ($x = 0, 0.15$) are investigated by Fe K-edge and As K-edge x-ray-absorption near-edge structure and extended x-ray-absorption fine structure from 10 to 300 K. A redistribution of electron density of state near the Fe site. It is found that the doping of Co introduces large static local lattice disorders of the As–Fe(Co) bonds. When we examine the local lattice structure around the Co dopants, we find the static local disorder is much more serious in the Co–As bonds comparing to that of As–Fe(Co) bonds. These facts suggest that strong electron-lattice interaction coexists with superconductivity in Fe-based superconductors.

1. Introduction

Materials with topological quantum states have been intensively investigated in the past over ten years due to their physical significance and potential application [1–4]. Among the various types of topological quantum materials, the topological superconductors have become the center of the unsolved issues in the topological research communities [5–7]. Topological superconductors have been proposed to be the best material platforms which harbour the long-sought yet elusive Majorana fermions, and can be exploited for fault-tolerant topological quantum computation. So far, two distinct approaches have been utilized to realize topological superconductivity. The first one is based on the proximity effect, where the superconductivity is produced locally at the interface between a topological insulator and a superconductor [8–10]. The second one is to obtain bulk superconductivity by tuning a topological insulator into superconducting state by carefully chosen element doping or intercalation [11–13]. However, controversies remain in both approaches, especially with regard to the observation of Majorana fermions.

Recently, it was proposed that some Fe-based superconductors have a metallic topologically nontrivial band structure, and host topological surface states near the Fermi energy [14]. This proposal is of unique importance since it could provide abundant material platforms for the investigation of topological superconductivity. Intriguingly, multiple signatures of topological superconductivity, such as the Majorana bound state and the metallic surface state with Dirac Fermions, have been observed in different types of Fe-based superconductors such as CaFeAsF and Fe(Te,Se) [15–19]. Comparing to the A$_x$Bi$_2$Se$_3$ (A = Cu, Sr, Nb) superconducting topological insulators, the relatively high transition temperature make the Fe-based superconductor a promising platform for studying the Majorana fermions and may further advance research on quantum computing. However, the multiband feature of Fe-based superconductors makes the electronic structures quite complicated, which deserve a systematic investigation. Local lattice structure is closely related to band splitting and thus can give valuable information on the band structure of such compounds. X-ray absorption
spectroscopy as a powerful tool to investigate the local lattice structure, has been widely utilized to probe the local electronic and lattice structures of several different types of Fe-based superconductors such as REFeAsO$_{1-x}$F$_x$ (RE = La, Sm, Nd, Pr, etc) and BaFe$_2$As$_2$ [20–25]. However, the investigations of the local lattice and electronic structure of CaFeAsF and Fe(Te,Se) by means of x-ray absorption spectroscopy measurements are still rare.

In this work, we examine the local electronic and lattice structures of CaFe$_{1-x}$Co$_x$AsF using the As and Fe K-edge x-ray absorption near-edge structure, as well as the As K-edge and Co K-edge extended x-ray absorption fine structure measurements. The combined experimental results indicate doping-induced local lattice distortions in the Fe(Co)-As bonds and a strong temperature-dependent redistribution of charge (a charge transfer from As to Fe sites). The present results suggest that the role of local lattice distortions could be important in the electronic properties in such compounds.

2. Experimental methods

The CaFe$_{1-x}$Co$_x$AsF ($x = 0, 0.15$) samples were prepared by a solid state reaction using high-purity Ca$_3$As$_2$, Fe$_3$As$_2$, Co$_3$As$_2$ and CaF$_2$ (powder, 99.999%, Alfa-Aesar) as starting materials. The starting material preparation procedures were carried out in an argon-filled glovebox (O$_2$, H$_2$O < 1 ppm). These materials were mixed in stoichiometric ratios, pressed, and heated in evacuated silica tubes at 1000 °C for 10 h to obtain sintered pellets. The lattice parameters as well as the basic electric and magnetic properties have been reported previously [26]. The parent compound CaFeAsF is not superconducting. With the incorporation of Co, the superconducting transition occurs. The superconducting transition temperature ($T_c$) is about 21 K in the $x = 0.15$ sample. X-ray absorption spectroscopy measurements were performed at the beamline BL13B of the Photon Factory, Tsukuba, Japan. The energy resolutions at the Fe K edge (7.11 keV) and As K edge (11.86 keV) were about 1 eV and 2 eV, respectively, using a double crystal Si(111) monochromator. The Fe K-edge and As K-edge data were sequentially recorded separately on slow heating. The helium cryostat mounted on a high-precision goniometer (Huber 420) was rotated to optimize the incidence angle.

3. Results and discussion

Figures 1(a) and (b) show the Fe K-edge x-ray absorption near-edge structure (XANES) spectra taken at different temperatures for the undoped CaFeAsF and Co-doped CaFe$_{1-x}$Co$_x$AsF ($x = 0.15$), respectively. The Fe K-edge XANES spectra exhibit several distinct band features, which are labeled as A, B, C, etc. Feature A locating at the pre-edge region is related to the excitations from the Fe 1s core level into the unoccupied 3d orbitals. The main absorption edge, features B and C, is ascribed to the excitations from the Fe 1s core level into the unoccupied 4p states. In order to see more clearly the energy shift with changing temperature in both samples, we plot the enlarged view of feature A in the insets of figures 1(a) and (b). From the inset of figure 1(a) it can be seen that the position of absorption threshold monotonously shifts to higher energy with decreasing temperature. The shift of absorption threshold towards higher energy implies the increase of energy difference between the core level and the unoccupied 3d states based on a dipole transition, due to the raising of the chemical potential of the unoccupied states. For the Co-doped sample, however, the energy shift is much weaker comparing to that of the undoped sample, suggesting that the chemical potential of the unoccupied states only exhibits small shift in the Co-doped sample.

The As K-edge XANES spectra for these samples at different temperatures are shown in figures 1(c) and (d). The As K-edge XANES spectra exhibit two predominant absorption edge features which are labeled as A and B. A remarkable contrast between the Fe K-edge and As K-edge spectra could be found in the temperature dependent energy shift, i.e., a positive shift in the Fe K-edge and a negative shift in the As edge with decreasing temperature. The negative energy shift in the As K-edge feature with decreasing temperature suggests the narrowing of energy difference between the core level and the unoccupied 4p states. It is also noticed that the narrowing of energy difference between the core level and the unoccupied 4p states is much weaker in the Co-doped sample compared to that in the parent compound CaFeAsF.

Figure 2(a) gives the energy shift of the Fe K-edge absorption thresholds as a function of temperature for the CaFeAsF as well as the CaFe$_{0.85}$Co$_{0.15}$AsF samples. For the CaFeAsF sample, the absorption threshold exhibits an energy shift of about 0.2 eV towards higher energy as the temperature is decreased from 300 K to 10 K. For the CaFe$_{0.85}$Co$_{0.15}$AsF sample, the Fe K-edge absorption threshold is about 0.26 eV lower at 300 K comparing to that of CaFeAsF. The lowering of the absorption threshold with Co doping is consistent with the introduction of electron charge carriers in CaFe$_{0.85}$Co$_{0.15}$AsF sample, where the energy difference between the Fe 1s core level and the unoccupied Fe 3d states is decreased. The energy shift of As K-edge absorption threshold is shown in figure 2(b). Different from those in Fe K-edge, the As K-edge absorption threshold exhibits an apparent energy
shift towards lower energy as the temperature is decreased in both CaFeAsF and CaFe_{0.85}Co_{0.15}AsF samples. It is worthwhile to note that in the undoped CaFeAsF, the energy shift in both the Fe and As K-edge thresholds exhibits a change of slope below 200 K, which is close to the temperature where the spin density wave instability occurs. In the CaFe_{0.85}Co_{0.15}AsF sample where the spin density wave instability is absent, there is no change of slope in energy shift of both the Fe and As K-edge threshold. Thus it is likely that the formation of spin density wave can substantially alter the positions of the x-ray absorption thresholds.

It is important to note that both the Fe K-edge and the As K-edge absorption thresholds substantially shift to lower energy in the Co-doped sample comparing to the undoped CaFeAsF, indicating that the unoccupied density of state decreases. This fact suggests that the electron-type charge carriers are introduced into both the Fe and As local states with the Co-doping. Figures 2(c) and (d) illustrate the energy differences of the Fe K-edge ($\Delta_{Fe}$) and the As K-edge ($\Delta_{As}$) and the energy difference between the Fe and As edge ($\Delta_{Fe} - \Delta_{As}$) of the CaFe_{1-x}Co_{x}AsF samples, respectively. Considering the substantial increase of $\Delta_{Fe}$ and decrease of $\Delta_{As}$ with decreasing temperature, the electron accumulation on the Fe site with decreasing temperature is implicated. A reversal of energy shift between the Fe and As K-edge absorption thresholds indicates a redistribution of electron density of state between Fe and As atoms. The electron density of state at the Fe site increases with decreasing temperature, suggesting temperature-dependent intra-layer charge redistribution. Similar temperature dependent electron dispersion was also found in Ba_{1-x}K_{x}Fe_{2}As_{2} [27]. The doped electrons might be accommodated in a particular electron pocket with an Fe atomic-orbital character at low temperature.

The As K-edge extended x-ray absorption fine structure (EXAFS) spectroscopy of the undoped CaFeAsF and the Co-doped CaFe_{0.85}Co_{0.15}AsF are measured from 5 K to 300 K. Figure 3(a) displays the representative As K-edge EXAFS spectra of the CaFe_{0.85}Co_{0.15}AsF sample measured at 10 K and 300 K. All spectra exhibit good statistics, which enable a reliable analysis of the local lattice structure. The As K-edge EXAFS oscillations (weighted by $k^2$) are extracted from the raw EXAFS spectra. Typical As K-edge EXAFS oscillations for the CaFe_{0.85}Co_{0.15}AsF sample are shown in figure 3(b). One can see that the magnitude of the oscillations decreases with increasing temperature, in accordance with the increased thermal disorder under high temperature.

Figure 3(c) shows the Fourier transforms [$\text{FT}(k^2 \chi (k))$] of the As K-edge EXAFS oscillations of the CaFe_{0.85}Co_{0.15}AsF sample from 300 K to 10 K. The Fourier transforms provide information on the atomic
distribution around the As site. One should be aware that the position of the peaks exhibited in the spectra do not appear at the actual bond distances because the actual distances should be corrected by the scattering phase shifts.

The Fourier transform peak appearing between 1.6–2.4 Å corresponds to the first-shell As–Fe bond distance. It can be clearly seen that the magnitude of the Fourier transform peak decreases with increasing temperature, suggesting an increased lattice disorder. In order to extract the local lattice structural information, the EXAFS signals of the first-shell As–Fe bond are separated from the other bond contributions and modeled in the single scattering approximation using the standard EXAFS equation \[ \chi(k) = \sum_i N_i S_i^2 f_i(k, R_i) e^{-2\Delta \delta_i} e^{-2k^2\sigma_i^2} \times \sin [2kR_i + \delta_i(k)], \]

where \( N_i \) is the number of the neighboring atoms at a bond distance \( R_i \), \( \delta_i \) is the phase shift, \( f_i(k, R_i) \) is the backscattering amplitude, \( \lambda \) is the photoelectron mean free path. The \( S_0^2 \) is the EXAFS amplitude reduction factor due to many-body effects related to the losses occurring during the photoelectron propagation in the material and the intrinsic losses due to shake-up and shake-off excitations created by the core hole in the absorption process, and \( \sigma_i^2 \) is the mean-square relative displacement (MSRD) parameter of the photo-absorber-backscatterer pairs. The ARTEMIS package with the amplitude and phase factors calculated by the FEFF is used in the fitting [28]. The effective number of neighboring Fe atoms \( (N_{Fe} = 4) \) is fixed during the fitting process.

Figure 3 (d) shows the comparison between the fitting curve and the experimental Fourier transform spectra of the CaFe\(_{0.85}\)Co\(_{0.15}\)AsF sample at 10 K. The fitting window is set to the \( R \) range between 1.6 and 2.4 Å, and the \( k \) range used in the fitting is 3–15 Å\(^{-1}\). It can be seen that the theoretical fitting can well reproduce the experimental data in the selected \( R \) range.

Figure 4 (a) gives the temperature dependence of the nearest-neighbor As–Fe(Co) bond distance of the CaFeAsF and CaFe\(_{0.85}\)Co\(_{0.15}\)AsF samples. In both samples, the As–Fe(Co) local bond distance systematically shrinks with decreasing temperature, without no anomaly. A remarkable feature is that the local As–Fe(Co) bond distance is substantially shorter in the Co-doped sample, comparing to that in the parent CaFeAsF sample. Considering the fact that the ionic radii of Co (0.745 Å) is greater than that of Fe (0.645 Å), the decrease of As–Fe...
(Co) bond distance cannot be simply explained by a rigid model. However, if we recall the situation in cuprate superconductor such as La$_{2-x}$Sr$_x$CuO$_4$, where the introduction of larger ions Sr$^{2+}$ for La$^{3+}$ leads to the decreases Cu–O bond distance, the decrease of As–Fe bond distance in Co-doped samples could be explained. In La$_{2-x}$Sr$_x$CuO$_4$, the corporation of Sr at the La site introduces efficient charge carriers into the Cu–O conductive plane, leading to an enhancement of the $pd\sigma$ hybridization of the Cu 3$d$ orbitals and O 2$p$ orbitals. The enhanced hybridization of the Cu and O orbitals causes the decrease of Cu–O local bond distance in La$_{2-x}$Sr$_x$CuO$_4$. In CaFe$_{1-x}$Co$_x$AsF, the introduction of Co also induces efficient charge carriers into the Fe(Co)–As conductive plane, leading to the enhancement of the $pd\sigma$ hybridization of the Fe(Co) 3$d$ orbitals and As 4$p$ orbitals. Thus it is

Figure 3. (a) Typical As K-edge EXAFS data measured using the fluorescence yield mode for the CaFeAsF at different temperature. (b) The As K-edge EXAFS oscillations extracted from (a). (c) The Fourier transforms of the As K-edge EXAFS (multiplied by $k^2$) for CaFeAsF at different temperature. The inset shows the peak height of the first-shell As–Fe correlation at different temperature. (d) A typical fitting to the As K-edge EXAFS data.

Figure 4. (a) Temperature dependence of As–Fe bond distance of the CaFeAsF and CaFe$_{0.85}$Co$_{0.15}$AsF samples. (b) The mean-square relative displacement for the two samples from 300 K to 5 K. The dashed lines are the fitting based on Einstein model.
The temperature dependences of the mean-square relative displacements ($\sigma^2$) of the As–Fe bond are shown in figure 4(b). The $\sigma^2$ values are larger in CaFe$_{0.85}$Co$_{0.15}$AsF than those in CaFeAsF parent compound, probably meaning a larger static lattice disorder in Co-doped samples. In order to get the quantitative information on the local lattice displacement of the two samples, we fit the temperature dependent $\sigma^2(T)$ using the Einstein model [28],

$$\sigma^2(T) = \frac{\hbar^2}{2k_B\mu \Theta_E} \cot \left( \frac{\Theta_E}{2T} \right) + \sigma_0^2,$$

where $\hbar$ is the reduced Planck constant, $k_B$ is the Boltzmann constant, $\mu$ is the reduced mass of the absorber-backscatterer pair, $\Theta_E$ is the Einstein temperature, and $\sigma_0^2$ represents the contribution from the static lattice disorder. For both samples, the experimental data can be well fitted using the Einstein model. The Einstein temperatures are found to be $\Theta_E = 283 \pm 5$ K in CaFeAsF and $\Theta_E = 236 \pm 4$ K in CaFe$_{0.85}$Co$_{0.15}$AsF, respectively. The Einstein temperatures in the CaFe$_{1-x}$Co$_x$AsF samples are relatively lower than those in Ca$_{0.9}$Pr$_{0.1}$Fe$_2$As$_2$ ($\Theta_E = 318 \pm 2$ K) and Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ ($\Theta_E = 308 \pm 17$ K) [29, 30]. These facts suggest that the vibration of Fe-As bond is larger in the CaFe$_{1-x}$Co$_x$AsF samples comparing to that in the so-called 122-phase Fe-based superconductors, probably indicating stronger electron-phonon coupling in CaFe$_{1-x}$Co$_x$AsF samples. It is also noticed that the Einstein temperature in CaFe$_{0.85}$Co$_{0.15}$AsF is lower than that in CaFeAsF, meaning that the electron-phonon coupling is stronger in the Co-doped samples comparing to the parent CaFeAsF. The static local lattice disorder $\sigma_0^2$ is $0.18 \times 10^{-3}$ Å$^2$ in CaFeAsF, while the $\sigma_0^2$ is significantly increased to $0.62 \times 10^{-3}$ Å$^2$ in CaFe$_{0.85}$Co$_{0.15}$AsF. The much larger As–Fe(Co) lattice disorder in the Co-doped samples might come from the mismatch in the As–Fe and As–Co bond distance.

In order to reveal the role of the incorporated Co atom on the enlarged static lattice disorder of the CaFe$_{0.85}$Co$_{0.15}$AsF sample, we perform the Co K-edge EXAFS measurements of the CaFe$_{0.85}$Co$_{0.15}$AsF sample from 300 K to 10 K. Figure 5(a) shows the typical Co K-edge EXAFS oscillations (weighted by $k^2$). The Co K-edge EXAFS oscillations exhibit good statistics in the whole temperature range, which the oscillation magnitude decreases with increasing temperature. Figure 2(b) gives the Fourier transforms of the Co K-edge EXAFS oscillations of the CaFe$_{0.85}$Co$_{0.15}$AsF sample from 300 K to 10 K. Here the Fourier transforms provide information on the atomic distribution around the doped Co atoms. In figure 5(b), the Fourier transform peak structure appearing between 1.6–2.7 Å contains two contributions: the nearest-neighboring Co–As and the next-nearest neighboring Co–Fe(Co) correlations. The Co K-edge EXAFS oscillations are modeled with two shells involving the nearest-neighboring Co–As and the next-nearest neighboring Co–Fe(Co) correlations. The typical fitting curve and the comparison with the experimental data are shown in figure 5(c). It is clear that the fitting curve can well reproduce the experimental data in the selected fitting window.

Figure 5(d) gives the temperature dependence of the local Co–As bond distance as well as the mean-square relative displacement of the Co–As bond. The local Co–As bond distance decreases with decreasing temperature, which is in accordance with the decreased As-Fe(Co) bond distance probed by the As K-edge EXAFS. At each temperature, the Co–As bond distance detected from Co K-edge EXAFS is very close to the As-Fe(Co) distance detected from As K-edge EXAFS, which also confirms the reliability of both the As K-edge and Co K-edge EXAFS data. The mean-square relative displacement also decreases with decreasing temperature. However, it is obvious that the value of the mean-square relative displacement of the Co–As bond is larger than that of the As-Fe(Co) bond. In order to quantitatively compare the mean-square relative displacements detected from the Co and As K-edge EXAFS, we fit the temperature dependence of $\sigma^2(T)$ of the Co–As bond using the Einstein model mentioned above. The fitting curve is plotted as the dashed line shown in figure 5(d). The Einstein temperature is determined to be $\Theta_E = 241 \pm 3$ K and the static local lattice disorder $\sigma_0^2$ is $1.17 \times 10^{-3}$ Å$^2$, respectively. Thus the Einstein temperature determined from the Co K-edge EXAFS is consistent with that determined from the As K-edge EXAFS. This is reasonable because the Einstein temperature reflects the intrinsic thermal properties of the sample itself. However, it is obvious that the static local lattice disorder of the Co–As bond is much larger than that of the As-Fe(Co) bond probed by As K-edge EXAFS. This fact suggests that the doped Co atoms introduce much more lattice disorders comparing to the original Fe atoms.

Both in cuprate and iron-based high temperature superconductors, the introduction of efficient charger carriers by element doping is the essential issue in the occurrence of superconductivity. However, whether or not the lattice effects are substantially involved in the superconducting mechanisms of high temperature superconductors has not reached a consensus. In CaFe$_{1-x}$Co$_x$AsF, we find that the local electron density of state is enhanced at low temperature, suggesting a charge density distribution between the local Fe and As sites. Importantly, we reveal a larger static local lattice disorder when the Co atoms are incorporated into the CaFe$_{1-x}$Co$_x$AsF compound. Consider that the incorporation of Co is an essential element in the occurrence of
superconductivity, the influence of local electron-lattice interaction should play substantial role in the electronic structures of the CaFe$_{1-x}$Co$_x$AsF compound.

4. Conclusions

In summary, we have investigated the local electronic and lattice structures of CaFe$_{1-x}$Co$_x$AsF ($x = 0, 0.15$) by means of temperature dependence of As and Fe $K$-edge x-ray absorption near edge structure as well as As and Co $K$-edge extended x-ray-absorption fine structure. With the incorporation of Co, the electron-type charge carriers are introduced into the Fe(Co)As planes. With decreasing temperature, we find an electron accumulation on the Fe site in CaFe$_{0.85}$Co$_{0.15}$AsF, leading to an increase of local electron density of state near the Fe site. Meanwhile, a large static local lattice disorder has been discovered near the Co site, meaning that the lattice effects must be taken into account in the electronic properties of CaFe$_{1-x}$Co$_x$AsF system.

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