



# Iron Isotope Effect and Local Lattice Dynamics in the (Ba, K)Fe<sub>2</sub>As<sub>2</sub> Superconductor Studied by Temperature-Dependent EXAFS

SUBJECT AREAS:

CONDENSED-MATTER  
PHYSICS

SUPERCONDUCTING PROPERTIES  
AND MATERIALS

THEORY AND COMPUTATION

QUANTUM MECHANICS

Wangsheng Chu<sup>1,2</sup>, Jie Cheng<sup>1,2</sup>, Shengqi Chu<sup>2</sup>, Tiandou Hu<sup>2</sup>, Augusto Marcelli<sup>4,1</sup>, Xianhui Chen<sup>3</sup> & Ziyu Wu<sup>1,2</sup>

Received  
9 October 2012

Accepted  
16 April 2013

Published  
29 April 2013

Correspondence and  
requests for materials  
should be addressed to  
Z.Y.W. (wuzy@ustc.  
edu.cn)

<sup>1</sup>National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P.R. China, <sup>2</sup>Beijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, P.R. China, <sup>3</sup>Hefei National Laboratory for Physical Science at Microscale and Department of Physics, University of Science and Technology of China, Hefei 230026, China, <sup>4</sup>Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, 00044 Frascati, Italy.

Currently available investigations of the isotope effect in Fe-based superconductors are all based on macroscopic resistivity and susceptibility measurements and results are highly controversial. Here we present an investigation of the Fe isotope effect in the (Ba, K)Fe<sub>2</sub>As<sub>2</sub> superconductor by temperature-dependent EXAFS in the framework of Einstein model. This method separates the static structural isotope contribution and the local lattice isotope contribution. Results point out the isotope substitution has a negligible effect on inter-atomic distances. On the contrary, both the local vibrations of the Fe-As and the Fe-Fe bonds show strong iron isotope dependence, which is a marker of an “intrinsic” isotope effect. This bulk iron isotope contribution to the local lattice dynamics suggests the local phonons play an important role in the (Ba, K)Fe<sub>2</sub>As<sub>2</sub> superconductor and a three-dimensional electron-phonon interaction should be considered to understand the superconducting mechanism of iron-based superconductors.

Since the discovery of cuprate superconductors in 1986, one of the still open and challenging problems in condensed matter physics is the origin of the superconductivity in high-temperature superconductors (HTSCs)<sup>1</sup>. Two decades of efforts based on thousands of experimental and theoretical researches pointed out that electron-electron interaction (EEI) rather than the electron-phonon interaction (EPI) plays the key role to trigger the superconductivity in HTSCs materials<sup>2,3</sup>. However, iron-based superconductors the new family of HTSCs discovered in 2008 does not show an agreement with this assumption<sup>4–6</sup>. Indeed, a clear iron isotope effect on T<sub>c</sub> was experimentally observed<sup>7–10</sup>. Chen *et al.*<sup>7</sup> firstly reported a large and positive iron isotope effect (Fe-IE) on the T<sub>c</sub> of both LnFeAs(O, F) and (Ba, K)Fe<sub>2</sub>As<sub>2</sub> superconductors. Khasanov *et al.*<sup>10</sup> found a larger Fe-IE exponent, well beyond the BCS value. Finally Shirage *et al.*<sup>8,9</sup> observed an inverse iron isotope effect in the (Ba, K)Fe<sub>2</sub>As<sub>2</sub> superconductor. Recently Yanagisawa *et al.*<sup>11</sup> presented a model explaining the sign inversion of the IE exponent. In his model, the (Ba, K)Fe<sub>2</sub>As<sub>2</sub> system is characterized by a multiband superconductivity originating by two different pairing channels: a phononic contribution and an antiferromagnetic (AF) fluctuation mechanism. However, his approach has been questioned by Bussmann-Holder and Keller<sup>12</sup> that claimed that an inversion of the Fe-IE exponent could not occur. More recently, Khasanov *et al.*<sup>13</sup> tried solving the discrepancy in the Fe-IE measurements by decomposing the exponent in two terms: one associated to structural changes and one intrinsic. They also pointed out that the Fe isotope substitution may induce small structural changes which, in turn, may affect T<sub>c</sub>. Actually, the controversy still on points out that:

- 1) lattice vibrations (i.e., phonons) play an important role in the superconductive mechanism(s) of iron-based superconductor materials;
- 2) the understanding of the IE in these iron-based materials remains a challenging issue to clarify.

Therefore, additional and more accurate experimental methods to measure the IE, probing not only macroscopic averaged properties such as those based on T<sub>c</sub> determinations, but also microscopic information of the system are required.



Here we present an investigation of the Fe-IE in the (Ba, K)Fe<sub>2</sub>As<sub>2</sub> superconductor system by temperature-dependent extended x-ray absorption spectroscopy (T-EXAFS). Due to the correlation between the absorber and the backscatter through the emitted photoelectrons excited by x-rays, EXAFS probes the local structure around the selected photoabsorber, such as the number of neighboring atoms  $N$ , the average bond length between absorbing atoms and neighboring atoms  $\langle r \rangle$  and the variance  $\sigma^2$ <sup>14,15</sup>. The Debye-Waller factor  $\sigma^2$  corresponds to the parallel mean square relative displacement (MSRD) among two atoms and it is the sum of two contributions:

$$\sigma^2 = \sigma_{stat}^2 + \sigma_{vib}^2. \quad (1)$$

The first term is temperature independent and associated to the static disorder, e.g., to the dispersion of bond lengths neglecting the vibrational dynamics. The second (dynamical) contribution is due to thermal vibrations and can be correlated to the vibrational spectrum of the system. The latter is usually well described by the Einstein model<sup>16</sup>

$$\sigma_{vib}^2 = \frac{\hbar^2}{2k\mu T_E} \coth \left[ \frac{T_E}{2T} \right]. \quad (2)$$

where  $\mu$  is the reduced mass of the atom pair,  $T$  is the temperature,  $k$  is Boltzmann's constant and  $\hbar$  is the Planck's constant. In the Eq. 2,  $T_E = (\hbar/k)\omega_E$  is the Einstein temperature and  $\omega_E$  is the corresponding Einstein frequency. The  $\sigma_{vib}^2$  contribution is different from zero also at 0 K.

Measurements of T-EXAFS may allow, via the analysis of the Debye-Waller factor, to separate the static and the thermal disorder contributions present in a sample. The first term is relative to the local structure and affects the electronic and the magnetic behavior of the system, while the second depends only by the local vibration behavior (i.e., phonons). By using the T-EXAFS technique, we may evaluate at the microscopic scale the contribution of the Fe-IE on both the static structure and the lattice dynamics in iron-based SCs. Because EXAFS is an element-specific technique, in these systems we may independently achieve information of the individual atomic pairs such as the Fe-As and the Fe-Fe pairs. Powder samples can be also used in an EXAFS experiment and single crystals are not necessary to accurately determine the mean-square relative displacement (MSRD).

Both Fe and As K-edge extended x-ray absorption fine structure spectra of the Ba<sub>0.6</sub>K<sub>0.4</sub>Fe<sub>2</sub>As<sub>2</sub> system by replacing <sup>56</sup>Fe (<sup>56</sup>Fe-sample) with the isotope <sup>54</sup>Fe (<sup>54</sup>Fe-sample) were measured vs. temperature down to 10 K. After an accurate analysis and comparison of EXAFS spectra of the two isotopic substitutions we point out that it does not induce detectable change of the average distances of both Fe-As and Fe-Fe atomic pairs while slightly modulates the Fe-As and Fe-Fe pair distributions. Moreover, it affects the local vibration of both Fe-As and Fe-Fe bonds.

## Results

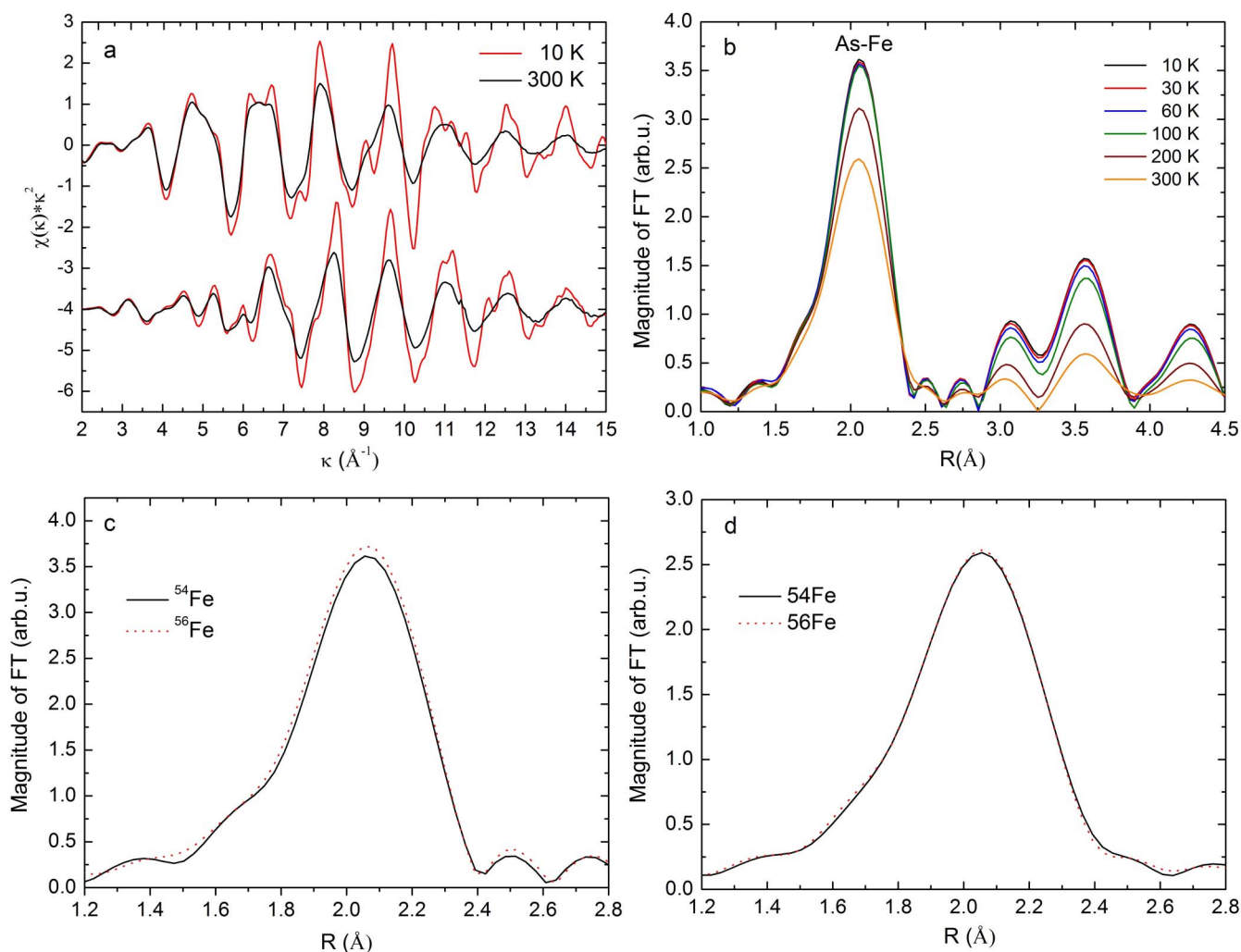
Fig. 1(a) compares As K-edge EXAFS data at 10 K and at room temperature (RT) showing a clear damping of the EXAFS oscillations vs. temperature. This behavior of the local structure is also clear looking at the comparison of the Fourier transforms (FTs) of the EXAFS spectra in Fig. 2(b). In this iron-based superconductor with the 122-structure no anomalies are detected at low temperatures, especially around  $T_c$ . In addition to our investigation, to our knowledge other two manuscripts published temperature-dependent EXAFS measurements on iron-based superconductors. They are from the Oyanagi and Tyson teams. Both investigated the (1111) iron-based superconductors LaFeAsO<sub>1-x</sub>F<sub>x</sub> obtaining different results. Oyanagi *et al.* found an anomalous behavior across  $T_{SDW}$  and  $T_c$ <sup>17</sup>. No such fine behavior has been observed in the data of Tyson<sup>18</sup>. We are convinced that in addition to always possible systematic errors or limited temperature points, the differences

observed can be associated to the different F concentration:  $x = 0.07$  and  $x = 0.11$ . Actually, the temperature-dependence of Fe-As and Fe-Fe MSRD of our system is similar to that observed by Tyson *et al.*, but our work is investigating a different type of iron-based superconductors: the (Ba, K)Fe<sub>2</sub>As<sub>2</sub> system belonging to the (122) family whose structure is well different from pnictides of the (1111) family. On the contrary, as we will discuss in the next, the iron isotope effect can be clearly seen looking at the magnitude of the FTs, which is correlated with the  $\sigma^2$  term, i.e., the EXAFS Debye-Waller (DW) factor.

In Fig. 1(c) and (d) we compare the first-shell peak (As-Fe pair) of the FTs of the <sup>54</sup>Fe- and <sup>56</sup>Fe-samples at 10 K and at RT, respectively. The position of the first-shell peak, i.e., the As-Fe pair in the FTs, is constant in the two samples and the same occurs for the Fe-Fe pair (panel d). Data point out that the Fe-IE does not affect the average distances of both Fe-As and Fe-Fe atomic pairs in the time-domain of the EXAFS experiments. A difference in the FTs associated to the isotopic substitution appears only looking at the magnitude of the first-shell peak. As it is well known, for a given crystal structure the magnitude of the FT peak depends by the  $\sigma^2$  term. As shown in Fig. 1(c) a difference in the FT magnitude for the As-Fe pair is evident at the lowest temperature (10 K - panel c). It gradually reduces with the temperature and at RT the two curves almost overlap (panel d). To obtain a quantitative dependence of  $\sigma^2$  vs.  $T$ , we extracted the DW of both As-Fe and Fe-Fe pairs by fitting EXAFS signals vs.  $T$  from 10 K to RT at both As and Fe K-edges, respectively. For the As K-edge, we considered the EXAFS signals of the nearest As-Fe bond. For the Fe K-edge, both nearest neighboring (Fe-As) and next-nearest neighboring (Fe-Fe) were filtered out. We have to underline here that the As-Fe correlation is identical to the Fe-As correlation in an EXAFS process. Therefore, in order to obtain exact information on the Fe-Fe bond we fix the distance and the DW factor of the Fe-As bond using parameters obtained by the As K-edge EXAFS fit during the analysis at the Fe K-edge EXAFS. Fig. 2a shows the quality of the EXAFS fit of the As K-edge EXAFS oscillations at RT. In Fig. 2b we compare the average distances of both Fe-As and Fe-Fe bonds of <sup>54</sup>Fe- and <sup>56</sup>Fe-samples, respectively, in the whole temperature range (10 ~ 300 K). Data are consistent with what showed in Fig 1c and 1d. We may emphasize that the result is different from the report of Khasanov *et al.*<sup>10</sup> on the FeSe<sub>1-x</sub> system that investigated the temperature dependence of the lattice structure by Neutron Powder Diffraction (NPD). This work also shows a large Fe-IE ( $\alpha_{Fe} = 0.81$ ) by means of SQUID measurements. As claimed by Khasanov *et al.*, it is the tiny modulation of the structural parameters caused by the isotope substitution that induces the large Fe-IE, beyond the framework of the BCS theory. However, these findings indicate that a Fe isotope effect on  $T_c$  is really present and related with the atomic or lattice structure in the Fe-based superconductors of the (11) family. In the superconductor (Ba, K)Fe<sub>2</sub>As<sub>2</sub> [(122) family] we detected an Fe-IE only on the atomic distributions and not on bond distances. Moreover, data points out that the isotope substitution has no effect on lattice distances in these samples of the (122) family. As a consequence, it represents an ideal model to characterize the isotope effect on the vibrational contributions, a fundamental issue to understand the electron-phonon interaction in a superconductor.

In Fig. 3 we also show the dependence of the DW factors of the As-Fe and the Fe-Fe bonds vs. temperature for both the <sup>54</sup>Fe- and <sup>56</sup>Fe-samples. A clear "isotopic" contribution appears at low temperature while at high temperature, the dependence of the DW factor approaches the classical linear behavior.

As outlined above, the  $\sigma^2$  term contains two contributions: the static disorder and the thermal disorder. In order to evaluate the contribution of the static disorder and of the vibrational frequency of the As-Fe and Fe-Fe bonds of isotopic substituted samples, we used the correlation Einstein model to fit the  $\sigma^2$  function vs. temperature:



**Figure 1 | Temperature-dependent EXAFS data for the Fe isotope substituted samples.** (a) Representative experimental EXAFS oscillations at the As (upper panel) and Fe (lower panel) K-edges of the  $^{54}\text{Fe}$ -sample. (b) FTs of the As K-edge EXAFS data measured cooling the sample down to 10 K. (c) Comparison between the first-shell peak of the FTs of the  $^{54}\text{Fe}$ - and  $^{56}\text{Fe}$ -samples at 10 K. (d) The same of (c) at RT.

$$\sigma^2(T) = \sigma_0^2 + \frac{\hbar^2}{2k\mu T_E} \coth\left[\frac{T_E}{2T}\right]. \quad (3)$$

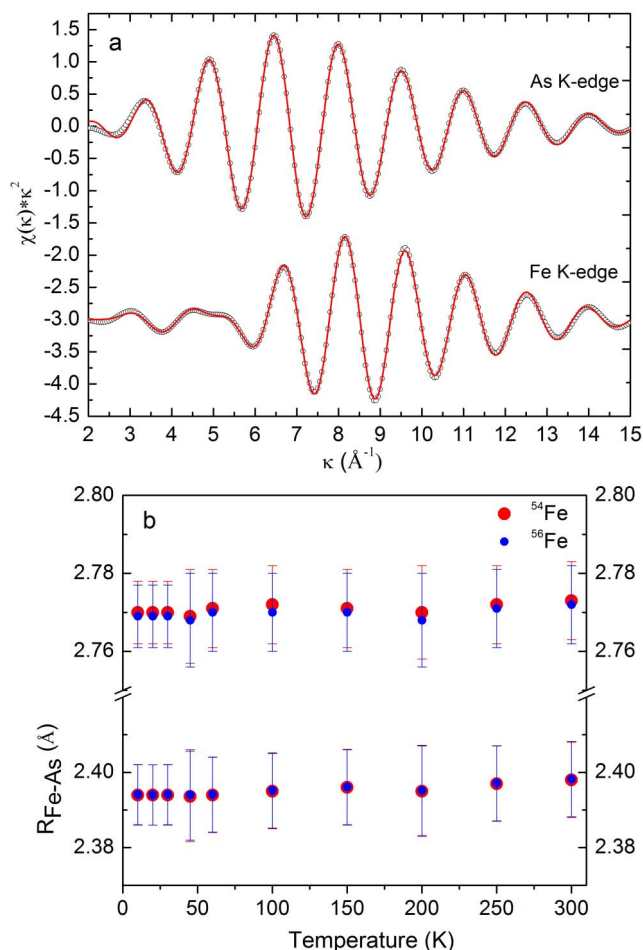
In Eq. 3  $\sigma_0^2$  is the static contribution to the bond and the quality of our simulations is shown by solid lines in the same figure. The corresponding values of the static contribution and of the vibrational frequency of the two samples are summarized in table 1 for both As-Fe and Fe-Fe bonds. Data show that the isotopic substitution gives rise to a weak modulation of the distribution of the interatomic distances of both Fe-As and Fe-Fe pairs. Moreover, the Fe-IE affects slightly more the static structural disorder of the Fe-Fe pair (it changes from 0.0056 to 0.0053  $\text{\AA}^2$ ) than that of the As-Fe (or Fe-As) pair that decreases from 0.0025 to 0.0023  $\text{\AA}^2$ . In addition, the static disorder of the Fe-Fe pair is much larger than that of the Fe-As pair. Bonds with a larger  $\sigma_0^2$  value (i.e., the Fe-Fe pair) and modulation due to the isotopic substitution, point out that these bonds are more flexible. This result is in agreement with other experimental data<sup>19</sup> and because decreasing temperature down to the structural transition temperature ( $T_s$ ) the Fe-Fe bond will undergo to a splitting<sup>20</sup>, data are also consistent with the occurrence of a structural phase transition in the iron layer of the  $\text{BaFe}_2\text{As}_2$  system. Also by using T-EXAFS technique, in the  $\text{K}_{0.8}\text{Fe}_{1.6}\text{Se}_2$  [122-chalcogenide] a similar lattice property has been detected. Also this work points out that the Fe-Fe bond is more flexible than the Fe-As bond<sup>21</sup>. The iron

isotope effect we observe on  $\sigma_0^2$  is due to the static structural modulation and corresponds to electronic and magnetic properties of the iron-based SCs.

A second important result we obtained by the analysis of the T-EXAFS experiments is that the Einstein temperature ( $T_E$ ) that is a probe of the vibrational frequency of the system, exhibits a shift for both the As-Fe and Fe-Fe bonds induced by the iron isotope substitution. The  $T_E$  of the As-Fe bond changes about 1.3% from 331.5 to 327.1 K after the substitution with  $^{54}\text{Fe}$  in the  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ . In the Fe-Fe bond,  $T_E$  shifts  $\sim 1.5\%$  from 169.0 to 166.5 K. Both Fe-Fe and Fe-As vibrations have then a similar, but not negligible contribution to the superconductive mechanism of iron-based SCs. Although the detected changes are small, similar changes of  $T_E$  occur for both Fe-Fe and Fe-As bonds. Actually, the Einstein temperature  $T_E$  can be associated to an effective force constant  $k_0$  normalized to the reduced mass  $\mu$ :

$$T_E = \sqrt{k_0/\mu}. \quad (4)$$

Actually, because the Einstein temperature is lower for the Fe-Fe bond, the latter is supposed to be softer than the Fe-As one. This experimental result points out a greater flexibility of the iron layers in the  $(\text{Ba}, \text{K})\text{Fe}_2\text{As}_2$  system. To evaluate the contribution of the isotope effect on the local vibration of the Fe-Fe and As-Fe correlations, we introduced the coefficient  $\alpha$

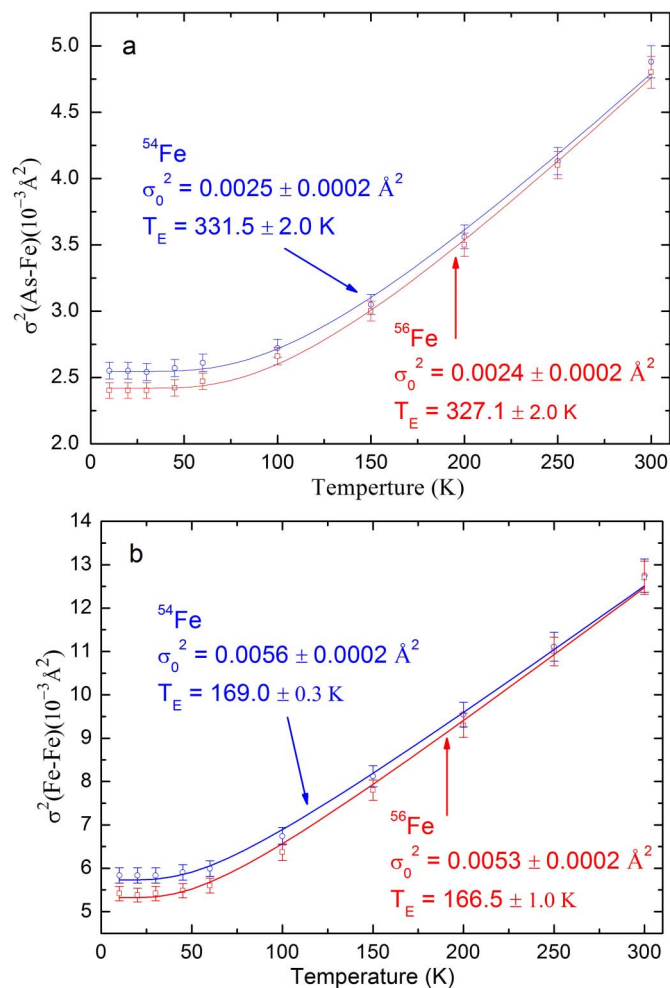


**Figure 2** | EXAFS fits and result of the bond distances vs. T. (a) Experimental (black circles) and fit (red lines) EXAFS oscillations of As-Fe (upper curve) and Fe-Fe (lower panel) shells, respectively, for the  $^{54}\text{Fe}$ -sample at RT. (b) Temperature dependence of Fe-As bond distances and Fe-Fe bond distances for the  $^{54}\text{Fe}$ - and the  $^{56}\text{Fe}$ -samples, respectively.

$$\alpha = -\frac{M}{\Delta M} \frac{\Delta T_E}{T_E} \quad (5)$$

very similar to the definition of the  $T_c$  isotope effect coefficient<sup>22</sup>. Here  $T_E$  is the Einstein temperature obtained by the EXAFS experiments, regarding both Fe-Fe and Fe-As bonds (Table 1) while  $M$  is the atomic mass of the isotopic substitution. Using the coefficient  $\alpha$  we may obtain an independent evaluation of the iron-isotope-effect for both As-Fe and Fe-Fe bonds. Using values listed in table 1 we got values of 0.37 and 0.41 for the As-Fe and Fe-Fe bonds, respectively, very close to the  $T_c$  iron-isotope-effect coefficient of 0.37 reported by the Chen's group<sup>7</sup>. Our analysis supports the hypothesis that the electron-phonon interaction plays a role in the superconductive mechanism of iron-based superconductors and that both Fe-Fe and Fe-As vibrations contribute to the superconducting mechanism.

Because Fe-Fe bonds lie in the superconducting layers ( $a$ - $b$  plane) while Fe-As bonds are oriented along the  $c$  axis, our result confirms in the iron-based superconductors the presence of a weak bulk iron isotope effect. In addition, it points out the presence in iron-based superconductors of a not negligible 3D electron-phonon interaction as shown in Fig. 4. This result can be also used to interpret the nearly isotropic superconducting properties of iron-based superconductors<sup>23</sup>, systems well different from layered cuprate superconductors.



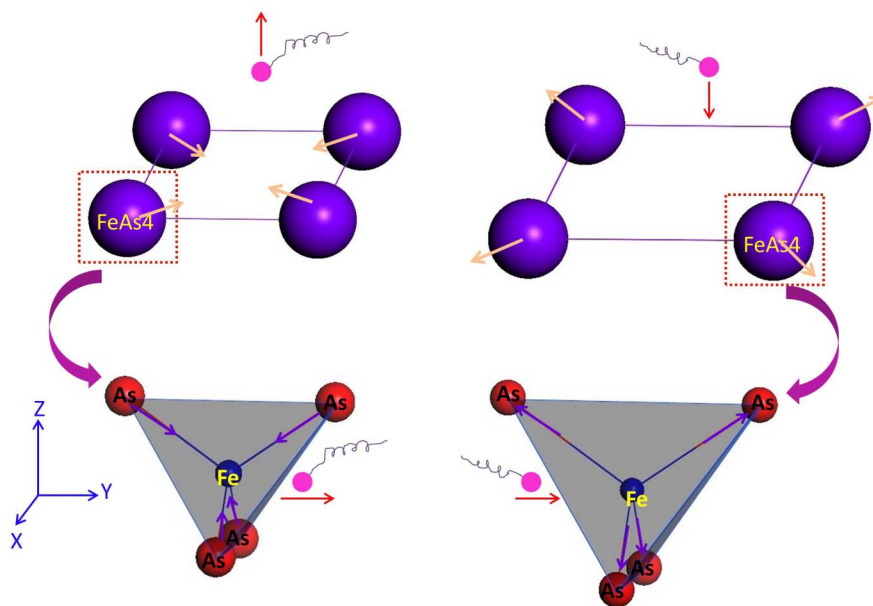
**Figure 3** | DW factors  $\sigma^2$  for the bond of the  $^{54}\text{Fe}$ - and the  $^{56}\text{Fe}$ -samples vs. T. (a) As-Fe bond; (b) Fe-Fe bond. Symbols are experimental data extracted from the EXAFS fits while solid lines are simulations based on the Einstein model. Bars refer to statistical errors.

## Discussion

An accurate EXAFS analysis of the  $(\text{Ba}, \text{K})\text{Fe}_2\text{As}_2$  system vs. temperature shows that an iron isotope effect correlated to the static structural distribution and with local vibrations can be detected. Changes of the static structural distribution may occur via changes of the inter-atomic distances and of the atomic distribution (or of the disorder). The Fe-IE does not induce appreciable changes in the inter-atomic distances while the atomic distribution is slightly affected. At present, it remains however extremely difficult identify a clear correlation among local disorder contributions (present in a powder sample) and superconducting mechanisms. In addition, we clearly showed the existence of a Fe-IE contribution to local vibrational term for both Fe-As and Fe-Fe bonds. Their isotopic exponents are in agreement with previous experiments<sup>7</sup> looking at the iron isotope

**Table 1** | Values of local static distortions and Einstein temperatures associated to the As-Fe and Fe-Fe bonds in the  $^{54}\text{Fe}$ - and  $^{56}\text{Fe}$ -samples

bonds	Isotope	$\sigma_0^2$ ( $\text{\AA}^2$ )	$T_E$ (K)	$\alpha$
As-Fe	$^{54}\text{Fe}$	$0.0025 \pm 0.0002$	$331.5 \pm 2.0$	0.37
	$^{56}\text{Fe}$	$0.0024 \pm 0.0002$	$327.1 \pm 2.0$	
Fe-Fe	$^{54}\text{Fe}$	$0.0056 \pm 0.0002$	$169.0 \pm 1.0$	0.41
	$^{56}\text{Fe}$	$0.0053 \pm 0.0002$	$166.5 \pm 1.0$	



**Figure 4 | Layout of Fe-Fe and Fe-As vibrations in the iron-based superconductors.** Fe-Fe bonds are in the superconducting layers and their vibrations attract electrons in the  $c$  direction, while Fe-As bonds are oriented along the  $c$  axis and their vibrations affect electrons in the  $a$ - $b$  layers.

effect in these systems. This result represents the first experimental link between the Fe-IE of  $T_c$  experiments and the superconducting mechanism at a microscopic level.

## Methods

Isotopically substituted polycrystalline samples were synthesized by the solid state reaction method described in detail in Ref. 7. Previous investigation of this superconductor showed a large iron isotope effect on the  $T_c$ . As and Fe K-edge absorption spectra were collected using a Si (111) double crystal monochromator at the XAFS station of the 1W1B beamline of the Beijing Synchrotron Radiation Facility (BSRF). The storage ring was working at 2.5 GeV with an electron current decreasing from 240 to 160 mA within about 8 hours. Samples were ground into fine powders and brushed onto tapes that were stacked together to give approximately one x-ray-absorption lengths at their corresponding metal edges. Samples were cooled by a closed-cycle helium refrigerator with an error bar on the temperature determination of about 0.1 K. Data were processed and analyzed using both UWXA<sup>24</sup> and FEFF 8.0 packages<sup>25,26</sup> to generate scattering amplitudes and phase shifts starting from available XRD refinements (see supplementary materials of Ref. 7).

1. Bednorz, J. G. & Müller, K. A. Possible high  $T_c$  superconductivity in the Ba-La-Cu-O system. *Z. Phys. B* **64**, 189–193 (1986).
2. Anderson, P. W. *Theory of Superconductivity in the High- $T_c$  Cuprates*. (Princeton University Press, Princeton, 1997).
3. Kresin, V., Morawitz, H. & Wolf, S. A. *Mechanism of Conventional and High  $T_c$  Superconductivity*. (Oxford Press, Oxford, 1993).
4. Kamihara, Y. *et al.* Iron-Based Layered Superconductor  $\text{La}[\text{O}_{1-x}\text{F}_x]\text{FeAs}$  ( $x = 0.05$ – $0.12$ ) with  $T_c \sim 26$  K. *J. Am. Chem. Soc.* **130**, 3296–3297 (2008).
5. Chen, X. H. *et al.* Superconductivity at 43 K in  $\text{SmFeAsO}_{1-x}\text{F}_x$ . *Nature* **453**, 761–762 (2008).
6. Takahashi, H. *et al.* Superconductivity at 43 K in an iron-based layered compound  $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$ . *Nature* **453**, 376–378 (2008).
7. Liu, R. H. *et al.* A large iron isotope effect in  $\text{SmFeAsO}_{1-x}\text{F}_x$  and  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ . *Nature* **459**, 64–67 (2009).
8. Shirage, P. M. *et al.* Inverse Iron Isotope Effect on the Transition Temperature of the  $(\text{Ba},\text{K})\text{Fe}_2\text{As}_2$  Superconductor. *Phys. Rev. Lett.* **103**, 257003 (2009).
9. Shirage, P. M. *et al.* Absence of an Appreciable Iron Isotope Effect on the Transition Temperature of the Optimally Doped  $\text{SmFeAsO}_{1-y}$  Superconductor. *Phys. Rev. Lett.* **105**, 037004 (2010).
10. Khasanov, R. *et al.* Iron isotope effect on the superconducting transition temperature and the crystal structure of  $\text{FeSe}_{1-x}$ . *New J. Phys.* **12**, 073024 (2010).
11. Yanagisawa, T. *et al.* Isotope Effect in Multi-Band and Multi-Channel Attractive Systems and Inverse Isotope Effect in Iron-Based Superconductors. *J. Phys. Soc. Jpn.* **78**, 094718 (2009).
12. Bussmann-Holder, A. & Keller, H. Comment on “Isotope Effect in Multi-Band and Multi-Channel Attractive Systems and Inverse Isotope Effect in Iron-Based Superconductors” *J. Phys. Soc. Jpn.* **79**, 126001 (2010).

13. Khasanov, R., Bendele, M., Bussmann-Holder, A. & Keller, H. Intrinsic and structural isotope effects in iron-based superconductors. *Phys. Rev. B* **82**, 212505 (2010).
14. Gregor, R. B. & Lytle, F. W. Extended x-ray absorption fine structure determination of thermal disorder in Cu: Comparison of theory and experiment. *Phys. Rev. B* **20**, 4902–4907 (1979).
15. Purans, J. *et al.* Isotopic Effect In Extended X-Ray-Absorption Fine Structure of Germanium. *Phys. Rev. Lett.* **100**, 055901 (2008).
16. Dalba, G. & Fornasini, P. EXAFS Debye-Waller Factor and Thermal Vibrations of Crystals. *J. Synchrotron Rad.* **4**, 243–255 (1997).
17. Zhang, C. J. *et al.* Low-temperature lattice structure anomaly in the  $\text{LaFeAsO}_{0.93}\text{F}_{0.07}$  superconductor by x-ray absorption spectroscopy: Evidence for a strong electron-phonon interaction. *Phys. Rev. B* **78**, 214513 (2008).
18. Tyson, T. A. *et al.* Temperature-dependent local structure of  $\text{LaFeAsO}_{1-x}\text{F}_x$ : Probing the atomic correlations. *J. Appl. Phys.* **108**, 123715 (2010).
19. Cheng, J. *et al.* Potassium doping effect on the lattice softening and electronic structure of  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$  probed by X-ray absorption spectroscopy. *J. Synchrotron Rad.* **17**, 730–736 (2010).
20. Rotter, M. *et al.* Spin Density Wave Anomaly at 140 K in the Ternary Arsenide  $\text{BaFe}_2\text{As}_2$ . *Phys. Rev. B* **78**, 020503(R) (2008).
21. Ladecola, A. *et al.* Large local disorder in superconducting  $\text{K}_{0.8}\text{Fe}_{1.6}\text{Se}_2$  studied by extended x-ray absorption fine structure. *J. Phys.: Condens. Matter* **24**, 115701 (2012).
22. Bill, A., Kresin, V. Z. & Wolf, S. A. *The Isotope Effect in Superconductors* (Review article), in *Pair Correlations in Many-Fermion Systems*, p. 25. (Plenum Press, 1998).
23. Yan, H. Q. *et al.* Nearly isotropic superconductivity in  $(\text{Ba},\text{K})\text{Fe}_2\text{As}_2$ . *Nature* **457**, 565–568 (2009).
24. Stern, E. A. *et al.* The UWXA<sup>24</sup> Analysis Package: Philosophy and Details. *Physica B* **208&209**, 117 (1995).
25. Rehr, J. J., Mustre de Leon, J., Zabinsky, S. I. & Albers, R. C. Theoretical x-ray absorption fine structure standards. *J. Am. Chem. Soc.* **113**, 5135–5140 (1991).
26. Zabinsky, S. I., Rehr, J. J., Ankudinov, A., Albers, R. C. & Eller, M. J. Multiple Scattering Calculations of X-ray Absorption Spectra. *Phys. Rev. B* **52**, 2995–3009 (1995).

## Acknowledgements

We thank Yi Luo, Yanin Xie, Jin Zhang, Liren Zheng for their valuable help and discussions. This work was partly supported by the National Outstanding Youth Fund (Project No. 10125523 to Z.Y.W.), the Knowledge Innovation Program of the Chinese Academy of Sciences (KJCX2-YW-N42) and the National Basic Research Program of China (2012CB825800). One of the authors (W.S.C.) thanks the Natural Science Foundation (11179023; 11275227) and the Fundamental Research Funds for the Central Universities (WK2310000019).

## Author contributions

Z.Y.W. designed the research. W.S.C. performed the experiment and analyzed the data, with the help from J.C. and S.Q.C. T.D.H. provided the support for the data collection and



analysis. W.S.C., A.M. and Z.Y.W. wrote the paper. X.H.C. provided the samples and discussed the results. All of the authors read and commended on the manuscript.

### **Additional information**

**Competing financial interests:** The authors declare no competing financial interests.

**License:** This work is licensed under a Creative Commons

Attribution-NonCommercial-NoDerivs 3.0 Unported License. To view a copy of this license, visit <http://creativecommons.org/licenses/by-nc-nd/3.0/>

**How to cite this article:** Chu, W.S. *et al.* Iron Isotope Effect and Local Lattice Dynamics in the (Ba, K)Fe<sub>2</sub>As<sub>2</sub> Superconductor Studied by Temperature-Dependent EXAFS. *Sci. Rep.* **3**, 1750; DOI:10.1038/srep01750 (2013).