SPECIAL TOPIC — High pressure physics

Structural stability at high pressure, electronic, and magnetic properties of BaFZnAs: A new candidate of host material of diluted magnetic semiconductors*

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The layered semiconductor BaFZnAs with the tetragonal ZrCuSiAs-type structure has been successfully synthesized. Both the *in-situ* high-pressure synchrotron x-ray diffraction and the high-pressure Raman scattering measurements demonstrate that the structure of BaFZnAs is stable under pressure up to 17.5 GPa at room temperature. The resistivity and the magnetic susceptibility data show that BaFZnAs is a non-magnetic semiconductor. BaFZnAs is recommended as a candidate of the host material of diluted magnetic semiconductor.

Keywords: diluted magnetic semiconductor, ZrCuSiAs-type structure, high pressure

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1. Introduction

The quaternary compound ZrCuSiAs has been reported by Johnson *et al.* since 1974, in which [ZrSi] layers and [CuAs] layers are stacked alternately along the *c*-axis, forming the tetragonal structure with the space group of $P4/nmm$.[1] Up to now, more than 150 compounds with the ZrCuSiAs-type structure have been synthesized.[2–5] These compounds have aroused a great deal of interest in recent years because of their rich physical properties.[5–9] The prominent example of such a case is, for instance, the parent compound of iron-based superconductors *Re*FeAsO (*Re* =rare earth metal). Spin density wave instability and structural transition exist in the system.[10–14] When charge carriers are doped into the parent compounds, the superconductivity emerges with the highest T_C up to 56 K.[14] These findings have stimulated enormous efforts to explore new superconductors and study the mechanism of superconductivity.

Recently, the successful discovery of diluted magnetic semiconductors (DMSs) in transition metal doped III–V semiconductors research has triggered extensive attention due to their potential applications for spin sensitive electronics.[15,16] However, in these typical III–V systems, such as (Ga, Mn)As, substitution of divalent Mn^{2+} into trivalent Ga^{3+} sites leads to severely limited chemical solubility, which resulted in high-quality metastable (Ga,Mn), as only available as epitaxial thin films. Meanwhile, the hetero-valent substitution, which simultaneously dopes both spin and carrier via magnetic atoms, makes it difficult to individually control charge and spin concentrations for better tuning of quantum freedom. To overcome these difficulties, exploring new bulk form DMSs with decoupled spin and carrier doping becomes necessary. After several years of efforts and studies, many bulk form DMSs with spin and charge decoupled doping, such as Li(Zn,Mn)*Pn* (*Pn* = As, P),[17,18] (Ba, K)(Zn, Mn)$_2$As$_2$,[19,20] (*R*, Na)(Zn, Mn)$_2$As$_2$ (*R* = Sr, Ca),[21,22] have been synthesized and extensively studied. The ZrCuSiAs-type compounds are expected to provide the opportunities to explore new DMSs because the doping of local moments and charge carriers can be decoupled in these compounds, which is feasible to optimize the Curie temperature.[23,24] (La, Ba)O(Zn, Mn)As is the first compound reported as the ZrCuSiAs-type DMS, in which the combination of the carrier doping via (La, Ba) substitution and spin doping via (Zn, Mn) substitution results in ferromagnetic order with Curie temperature (T_C) up to $\sim$ 40 K.[23] Shortly after this, several more DMSs with ZrCuSiAs-type structure were reported, such as (La, Sr)O(Cu, Mn)S[24] and (La, Ca)O(Zn, Mn)Sb.[25]

In this paper, we report the synthesis of a high-quality compound BaFZnAs and its crystal structural stability under high pressure, resistivity ρ, specific heat, and magnetism. It is recommended as a new attractive candidate for finding a new DMS.

2. Experimental details

High-quality polycrystalline BaFZnAs sample was synthesized by the solid-state reaction method, of which the

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scanning electron microscope (SEM) image was shown in Fig. 1(c). The precursor BaAs was first synthesized by heating Ba flakes (purity 99.9%) and As power (purity 99.99%) at 800 °C for 10 h in an evacuated quartz tube. Then the starting material BaF_2 (purity 99.9%), BaAs, Zn power (purity 99.99%), and As power were mixed together according to the stoichiometric ration of BaFZnAs, ground, and then pressed into pellets in a glove box. The pellets were loaded into an alumina crucible and sealed in Nb tube under one atm of Argon gas. This Nb tube was then sealed in a quartz tube under a vacuum. The sample was heated to 900 °C (120 °C h^{-1}) for 20 h. The sample was ground and re-pelletized for the second heat treatment at 900 °C for another 20 h. The BaFZnAs compound is not sensitive to the dry air.

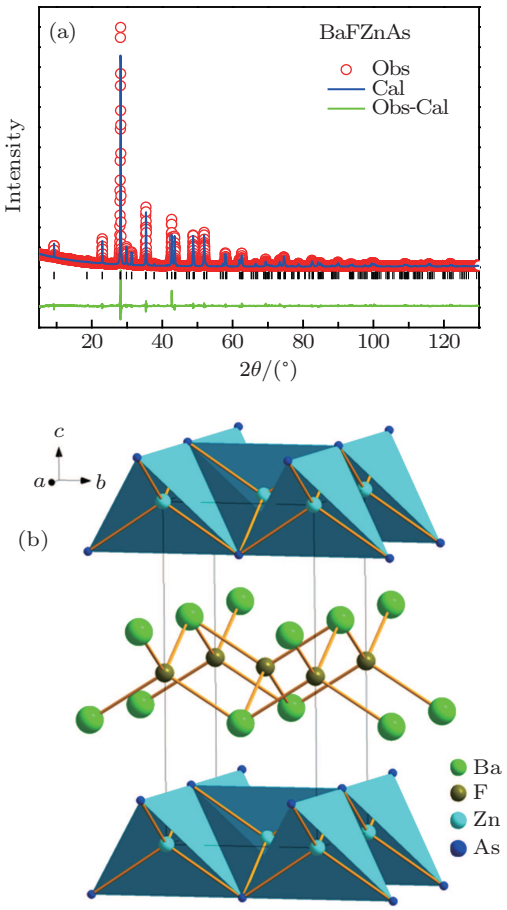


Fig. 1. (color online) (a) The x-ray diffraction of BaFZnAs at ambient pressure. (b) The crystal structure of BaFZnAs. (c) Scanning electron microscope (SEM) of BaFZnAs.

The x-ray diffraction at ambient pressure was carried out on a Philips X'pert diffractometer using the Cu-$K\alpha$ radiation. The refinement was performed by the Rietveld method using the software package PC-GSAG.[26] The x-ray diffraction experiments at high pressure were performed at Advanced Photon Source (APS) in America with a wavelength of 0.4199 Å. High-pressure Raman experiments were carried out using the high-pressure assembly of a diamond anvil cell (DAC) with silicone oil as the pressuretransmitting medium. Raman spectra were collected in backscattering geometry on the Renishaw Micro-Raman Spectroscopy System with a laser wavelength of 532 nm and an output power of 100 mW.

The resistivity and specific heat were measured on a Quantum Design PPMS. The DC-susceptibility measurement was performed on a Quantum Design superconducting quantum interference device (SQUID VSM) under an applied field of 0.1 T in the temperature ranging from 5 K to 300 K.

3. Results and discussion

Figure 1(a) shows the x-ray diffraction pattern of BaFZnAs at ambient pressure, which is refined based on the tetragonal ZrSiCuAs-type structure with space group $P4/nmm$. The crystal structure is similar to that of LaOFeAs,[13] LaOZnAs,[27,28] LaOCuS,[29,30] and LaOZnSb.[31,32] LaOFeAs is a typical parent compound of the "1111"-type iron-based pnictide superconductor, whereas the other three compounds are the host materials of the "1111"-type DMSs. The Rietveld refinement is smoothly converged to $R_p = 5.9\%$ and $wR = 7.9\%$. A summary of the crystallographic data is presented in Tables 1 and 2. The obtained lattice parameters for BaFZnAs are $a = b = 4.2351$ Å and $c = 9.5431$ Å, which are consistent with the previously reported values ($a = 4.2383$ Å and $c = 9.5260$ Å),[33] and larger than that of LaOZnAs ($a = 4.1049$ Å and $c = 9.0818$ Å).[27] The crystal structure of BaFZnAs consists of alternating $[BaF]^+$ and $[ZnAs]^-$ layers with edge-sharing FBa_4 and $ZnAs_4$ tetrahedral shown in Fig. 1(b), which is similar to the iron pnictide superconductors parent compound SrFFeAs.[34]

Table 1. Summary of crystallographic data for BaFZnAs.

Compound	BaFZnAs
Crystal system	tetragonal
Space group	$P4/nmm$ (No. 129)
Formula weight/g·mol^{-1}	604.659
Calculated density/g·cm^{-3}	5.866
Lattice parameters	
a/Å	4.23518(42)
c/Å	9.5431(114)
Cell volume/Å	171.173(3)
Formula units per cell, Z	2
R_p, wR_p	0.0591,0.0791
Goodfit	5.503

Table 2. Position coordinates and thermal parameters for BaFZnAs.

Atom	Wyck	x	y	z
Ba	2c	0.2500	0.2500	0.1477
F	2a	0.7500	0.2500	0.0000
Zn	2b	0.7500	0.2500	0.5000
As	2c	0.2500	0.2500	0.6545

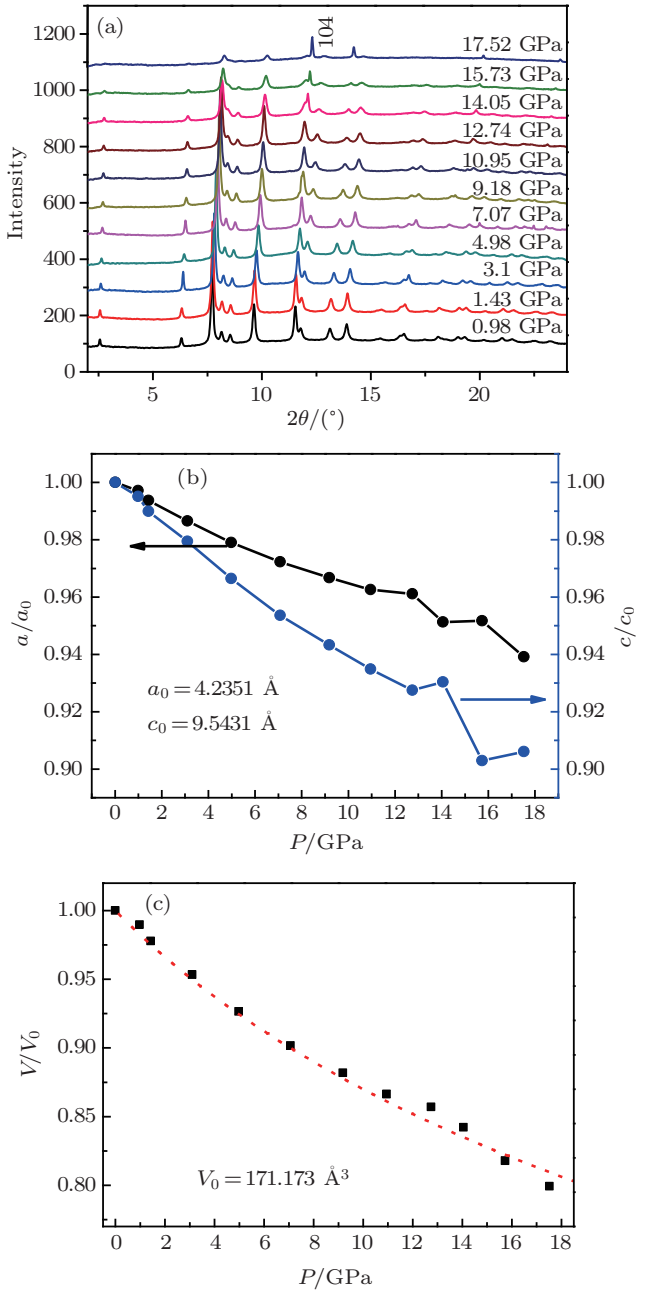


Fig. 2. (color online) (a) The synchrotron x-ray diffraction patterns for BaFZnAs at different high pressures. (b) Pressure dependence of lattice parameters. (c) Pressure dependence of the crystal cell volume.

To further study the structure stability of BaFZnAs under high pressure, *in-situ* high-pressure synchrotron x-ray diffraction experiments were performed using DAC with pressure up to 17.5 GPa. Figure 2(a) shows the diffraction patterns of BaFZnAs at different pressures. All the peaks shift to higher angles as pressure increases, while structure remains strictly unchanged up to 17.5 GPa. The lattice parameters of the BaFZnAs samples at different pressures were obtained from the profile fit of the synchrotron x-ray diffraction. Figure 2(b) presents the pressure dependence of lattice parameters of BaFZnAs. The lattice parameters a and c smoothly decrease by 6.1% and 9.4%, respectively, with respect to the increasing pressure to 17.5 GPa. This clearly indicates that the c axis is relatively easier to be compressed compared to the a axis. For the compounds with a layered structure similar to BaFZnAs, the shape of the edge-sharing tetrahedral is easy to be changed by pressure and suddenly collapses at a critical pressure but keeping the space group, which is the so called isostructural phase transition. For example, the iron-based superconductor Nd(O, F)FeAs undergoes an isostructural phase transition at about 10 GPa, where the lattice constants change suddenly and the volume of crystal cell collapses.[35] However, for BaFZnAs, no anomaly can be found in the pressure dependence of a and c axis and the crystal cell volume, which indicates that the structure of BaFZnAs is stable within this pressure range.

Figure 2(c) shows the pressure P versus V/V_0 curve. The Birch–Murnaghan equation is used to deduce the bulk modules B_0 for BaFZnAs,

$$P\,(\mathrm{GPa}) = \frac{3}{2}B_0\left[\left(\frac{V_0}{V}\right)^{7/3} - \left(\frac{V_0}{V}\right)^{5/3}\right] \times \left\{1 - \left(3 - \frac{3}{4}\times B_0'\right)\times\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]\right\}.$$

The pressure derivative B_0' is fixed as 4 and the fitting result gives the value of bulk modulus $B_0 = 56$ GPa, which is comparable with the similar layered compounds LiFeAs[36] and NaFeAs.[37] It indicates that BaFZnAs is a relatively soft material.

Raman spectroscopy is a powerful tool to detect the phase transition or electronic structure changes.[38,39] High-pressure Raman scattering measurement has been performed on the BaFZnAs compound with increasing pressure from 0.08 GPa to 21.71 GPa. As shown in Fig. 3(a), the characteristic Raman spectra of this compound are comprised of four major modes at 124.3 cm^{-1}, 178.6 cm^{-1}, 207.8 cm^{-1}, 316.5 cm^{-1}, and a few other small peaks. The figure also shows no sign of new peak appearance up to the highest pressure, which is consistent with the result of high-pressure x-ray diffraction and demonstrates the structural stability. As the pressure increases, the Raman modes of BaFZnAs shift to higher frequencies due to the fact that the structure of the compound becomes more compact and the bond distances are shortened. However, the pressure dependence of the Raman scattering of the BaFZnAs compound is anisotropic and the four major characteristic modes have different pressure coefficients. As shown

in Fig. 3(b), for the BaFZnAs compound, the pressure coefficient is about 4.1 and 2.0 for the 207.8 cm^{-1} mode and that of 124.3 cm^{-1} mode, respectively. The pressure coefficient for the 207.8 cm^{-1} mode is two times larger than the 124.3 cm^{-1} mode.

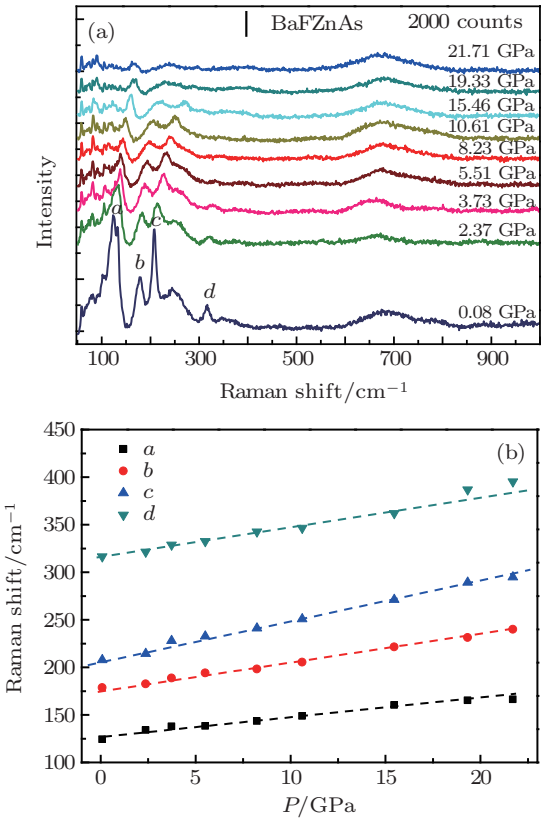


Fig. 3. (color online) (a) High-pressure Raman spectra of BaFZnAs with the pressure ranging from 0.08 GPa to 21.71 GPa. (b) Pressure dependence of Raman mode shifts for BaFZnAs compound.

The temperature dependence of resistivity of BaFZnAs is shown in Fig. 4. The resistivity increases with decreasing temperature, demonstrating a semiconducting behavior. As it is known, the [FeAs] layers in the iron-based superconductors are the conducting layers because the 3d-band derived from Fe crosses the Fermi surface.[40,41] If the ions Fe^{2+} in the [FeAs] layers were replaced by ions Zn^{2+}, the Zn-based compounds would become semiconductors for the d^{10} configure of Zn^{2+}. Therefore, BaFZnAs derived from SrFFeAs is a semiconductor. The resistivity of BaFZnAs at room temperature is about 3.6 MΩ·mm, which is much larger than that of $BaZn_2As_2$, which is the hostmaterial of DMS.[19] The inset of Fig. 4 shows the resistivity plotted in log scale $\ln\rho$ versus $1/T$, with the fit of $\sigma(T) = \sigma_0 \exp(-E_a/k_B T)$, where σ_0 is the preexponential constant, k_B is the Boltzmann constant, and E_a is the activation energy. The value of E_a from the fitting is 0.43 eV, i.e., bang gap $E_g = 2E_a = 0.86$ eV. The band gap is larger than that ($E_g = 0.23$ eV) of $BaZn_2As_2$,[42] suggesting a larger ionicity than that of $BaZn_2As_2$.

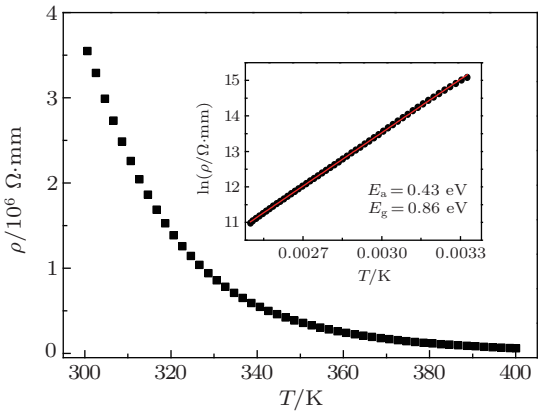


Fig. 4. (color online) (a) Temperature dependence of resistivity $\rho(T)$ for BaFZnAs. The inset shows $\ln(\rho)$ versus inverse temperature T^{-1}.

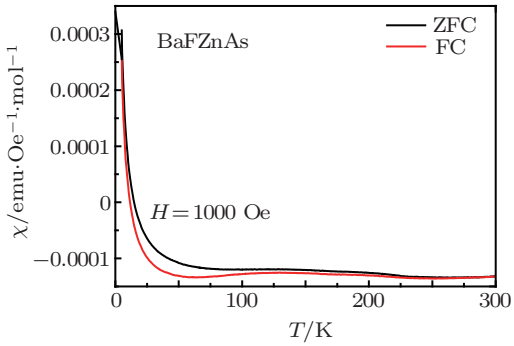


Fig. 5. (color online) Temperature dependence of susceptibility in zero-field-cooling (ZFC) and field cooling (FC) modes under $H = 1000$ Oe for BaFZnAs.

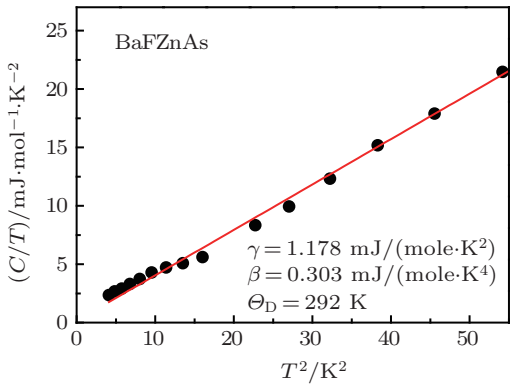


Fig. 6. (color online) The specific heat data of C/T versus T^2 at low temperature of BaFZnAs.

The temperature dependence of the susceptibility of BaFZnAs is presented in Fig. 5. No magnetic phase transition is found in the susceptibility curve. Because all the electrons in the compound are paired, the susceptibility is diamagnetic in the temperature range from 15 K to 300 K. The positive magnetic susceptibility in low temperature results from the paramagnetic intrinsic impurity. Specific heat (SH) measurement was preformed and the result is shown in Fig. 6. Because BaFZnAs is nonmagnetic, the magnetic contribution to the specific heat can be ignored. The low-temperature heat capacity follows the function $C_V = \gamma T + \beta T^3$, where γ

and β are the coefficient of electron SH and phonon SH, respectively. By fitting the data, they were calculated to be $\gamma = 1.178$ mJ/(mol·K^2) and $\beta = 0.303$ mJ/(mol·K^4). The small value of γ suggests that the electron SH contribution near the Fermi surface can also be ignored, which demonstrates that there are a few charge carriers in BaFZnAs, consistent with the results of the resistivity measurement. The Debye temperature Θ_D is about 292 K deduced from β and the value is comparable with the similar compound LaOFeAs.[43]

From the above results, it can be concluded that BaFZnAs is a non-magnetic semiconductor with a layered structure. $BaZn_2As_2$ with [ZnAs] layers has been found to be the host material of DMS and the highest Curie temperature is up to 230 K in $(Ba_{0.7}K_{0.3})(Zn_{0.85}Mn_{0.15})_2As_2$.[19] Similar to the $BaZn_2As_2$ system, the ions of Ba and Zn in the BaFZnAs compound are expected to be substituted with ions K and Mn separately to induce charge carriers and local moment, which may result in long-range ferromagnetic order. We are currently working on these dopings to show this behavior. BaFZnAs is recommended to be another candidate of host material of DMS.

4. Conclusions

In conclusion, we have synthesized the compound of BaFZnAs. It crystallizes into a layered tetragonal structure with a space group of $P4/nmm$ and the structure is stable under pressure up to 17.5 GPa. This compound is a relatively soft material with the bulk modulus $B_0 = 56$ GPa. BaFZnAs shows a non-magnetic performance with $E_g = 0.86$ eV. The layered compound of BaFZnAs is a candidate of host material of diluted magnetic semiconductor, in which the local moment and charge carrier could be separately doped to form a new DMS.

References

[1] Johnson V and Jeitschko W 1974 *J. Solid State Chem.* **11** 161
[2] Palazzi M, Carcaly C and Flahaut J 1980 *J. Solid State Chem.* **35** 150
[3] Palazzi M and Jaulmes S 1981 *Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry* **37** 1337
[4] Nientiedt A T, Jeitschko W, Pollmeier P G and Brylak M 1997 *Zeitschrift für Naturforschung B* **52** 560
[5] Poettgen R and Johrendt D 2008 *Z. Naturforsch.* **63b** 1135
[6] Kabbour H, Cario L and Boucher F 2005 *J. Mater. Chem.* **15** 3525
[7] Zhao L D, Berardan D, Pei Y L, Byl C, Pinsard-Gaudart L and Dragoe N 2010 *Appl. Phys. Lett.* **97** 092118
[8] Matsuishi S, Inoue Y, Nomura T, Hirano M and Hosono H 2008 *J. Phys. Soc. Jpn.* **77** 113709
[9] Wang X C, Liu Q Q, Lv Y X, Gao W B, Yang L X, Yu R C, Li F Y and Jin C Q 2008 *Solid State Commun.* **148** 538
[10] Li Y K, Xu X F, Cao C, Shen C Y, Luo Y K, Tao Q, Lin X, Zhang L, Cao G H and Xu Z A 2012 *Phys. Rev. B* **86** 104408
[11] Chen X H, Wu T, Wu G, Liu R H, Chen H and Fang D F 2008 *Nature* **453** 761
[12] Chen G F, Li Z, Wu D, Dong J, Li G, Hu W Z, Zheng P, Luo J L and Wang N L 2008 *Phys. Rev. Lett.* **100** 247002
[13] Kamihara Y, Watanabe T, Hirano M and Hosono H 2008 *J. Am. Chem. Soc.* **130** 3296
[14] Ren Z A, Yang J, Lu W, Yi W, Shen X L, Li Z C, Che G C, Dong X L, Sun L L, Zhou F and Zhao Z X 2008 *Europhys. Lett.* **82** 57002
[15] Ohno H 1998 *Science* **281** 951
[16] Dietl T 2010 *Nat. Mater.* **9** 965
[17] Deng Z, Jin C Q, Liu Q Q, Wang X C, Zhu J L, Feng S M, Chen L C, Yu R C, Arguello C, Goko T, Ning F L, Zhang J S, Wang Y Y, Aczel A A, Munsie T, Williams T J, Luke G M, Kakeshita T, Uchida S, Higemoto W, Ito T U, Gu B, Maekawa S, Morris G D and Uemura Y J 2011 *Nat. Commun.* **2** 422
[18] Deng Z, Zhao K, Gu B, Han W, Zhu J L, Wang X C, Li X, Liu Q Q, Yu R C, Goko T, Frandsen B, Liu L, Zhang J S, Wang Y Y, Ning F L, Maekawa S, Uemura Y J and Jin C Q 2013 *Phys. Rev. B* **88** 081203(R)
[19] Zhao K, Deng Z, Wang X C, Han W, Zhu J L, Li X, Liu Q Q, Yu R C, Goko T, Frandsen B, Liu L, Ning F L, Uemura Y J, Dabkowska H, Luke G M, Luetkens H, Morenzoni E, Dunsiger S R, Senyshyn A, Boni P and Jin C Q 2013 *Nat. Commun.* **4** 1442
[20] Zhao K, Chen B J, Zhao G Q, Yuan Z, Liu Q Q, Deng Z, Zhu J L and Jin C Q 2014 *Chin. Sci. Bull.* **59** 2524
[21] Chen B J, Zhao K, Deng Z, Han W, Zhu J L, Wang X C, Liu Q Q, Frandsen B, Liu L, Cheung S, Ning F L, Munsie T J S, Medina T, Luke G M, Carlo J P, Munevar J, Uemura Y J and Jin C Q 2014 *Phys. Rev. B* **90** 155202
[22] Zhao K, Chen B J, Deng Z, Han W, Zhao G Q, Zhu J L, Liu Q Q, Wang X C, Frandsen B, Liu L, Cheung S, Ning F L, Munsie T J S, Medina T, Luke G M, Carlo J P, Munevar J, Zhang G M, Uemura Y J and Jin C Q 2014 *J. Appl. Phys.* **116** 163906
[23] Ding C, Man H Y, Qin C, Lu J C, Sun Y Y, Wang Q, Yu B Q, Feng C M, Goko T, Arguello C J, Liu L, Frandsen B J, Uemura Y J, Wang H D, Luetkens H, Morenzoni E, Han W, Jin C Q, Munsie T, Williams T J, D'Ortenzio R M, Medina T, Luke G M, Imai T and Ning F L 2013 *Phys. Rev. B* **88** 041102
[24] Yang X J, Li Y K, Shen C Y, Si B Q, Sun Y L, Tao Q, Cao G H, Xu Z and Zhang F C 2013 *Appl. Phys. Lett.* **103** 022410
[25] Han W, Zhao K, Wang X C, Liu Q Q, Ning F L, Deng Z, Liu Y, Zhu J L, Ding C and Man H Y 2013 *Sci. China Phys. Mechanics and Astronomy* **56** 2026
[26] Larson A C and Von Dreele R B 1994 *General Structure Analysis System*. Los Alamos National Laboratory Report: LAUR 86-748
[27] Takano Y, Komatsuzaki S, Komasaki H, Watanabe T, Takahashi Y and Takase K 2008 *J. Alloy. Compd.* **451** 467
[28] Nientiedt A T and Jeitschko W 1998 *Inorg. Chem.* **37** 386
[29] Palazzi P and Acad C R 1981 *Sc. Ser. II* **292** 789
[30] Koyano S, Takase K, Kuroiwa Y, Aoyagi S, Shoji O, Sato K, Takahashi Y and Takano Y Sekizawa K 2006 *J. Alloy. Compd.* **95** 408
[31] Schellenberg I, Nilges T and Pöttgen R 2008 *Z. Naturforsch.* **63b** 834
[32] Wollesen P, Kaiser J W and Jeitschko W 1997 *Z. Naturforsch.* **52b** 1467
[33] Charkin D O, Urmanov A V, Plokhikh I V, Korshunov A D, Kuznetsov A N and Kazakov S M 2014 *J. Alloy. Comp.* **585** 644
[34] Han F, Zhu X Y, Mu G, Cheng P and Wen H H 2008 *Phys. Rev. B* **78** 180503(R)
[35] Zhao J G, Wang L H, Dong D W, Liu Z G, Liu H Z, Chen G F, Wu D, Luo J L, Wang N L, Yu Y, Jin C Q and Guo Q Z 2008 *J. Am. Chem. Soc.* **130** 13828
[36] Mito M, Pitcher M J, Crichton W, Garbarino G, Baker P J, Blundell S J, Adamson P, Parker D R and Clarke S J 2009 *J. Am. Chem. Soc.* **131** 2986
[37] Liu Q Q, Yu X H, Wang X C, Deng Z, Lv Y X, Zhu J L, Zhang S J, Liu H Z, Yang W G, Wang L, Mao H, Shen G Y, Lu Z Y, Ren Y, Chen Z Q, Lin Z J, Zhao Y S and Jin C Q 2011 *J. Am. Chem. Soc.* **133** 7892
[38] Hadjiev V, Iliev M, Sasmal K, Sun Y Y and Chu C 2008 *Phys. Rev. B* **77** 220505(R)
[39] Zhang L, Fujita T, Chen F L, Feng D, Maekawa S and Chen M W 2009 *Phys. Rev. B* **79** 052507
[40] Kuroki K, Onari S, Arita R, Usui H, Tanaka Y, Kontani H and Aoki H 2008 *Phys. Rev. Lett.* **101** 081007
[41] Mazin I I, Singh D J, Johannes M D and Du M H 2008 *Phys. Rev. Lett.* **101** 057003
[42] Xiao Z, Hiramatsu H, Ueda S, Toda Y, Ran F Y, Guo J, Lei H, Matsuishi S, Hosono H and Kamiya T 2014 *J. Am. Chem. Soc.* **136** 14959
[43] McElroy C A, Hamlin J J, White B D, McGuire M A, Sales B C and Maple M B 2013 *Phys. Rev. B* **88** 134513