Electronic structure of YFe$_2$Ge$_2$ studied by angle-resolved photoemission spectroscopy

D. F. Xu,$^{1,2,3}$ D. W. Shen,$^{4,5,†}$ D. Zhu,$^6$ J. Jiang,$^{1,2,3}$ B. P. Xie,$^{1,2,3}$ Q. S. Wang,$^1$ B. Y. Pan,$^1$ P. Dudin,$^7$ T. K. Kim,$^7$ M. Hoesch,$^7$ J. Zhao,$^{1,3}$ X. G. Wan,$^6$ and D. L. Feng,$^{1,2,3,†}$

$^1$State Key Laboratory of Surface Physics, Department of Physics, Fudan University, Shanghai 200433, China
$^2$Laboratory of Advanced Materials, Fudan University, Shanghai 200433, China
$^3$Collaborative Innovation Center of Advanced Microstructures, Fudan University, Shanghai 200433, China
$^4$State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Microsystem and Information Technology (SIMIT), Chinese Academy of Sciences, Shanghai 200050, China
$^5$CAS-Shanghai Science Research Center, Shanghai 210203, China
$^6$National Laboratory of Solid State Microstructures, Collaborative Innovation Center of Advanced Microstructures, and College of Physics, Nanjing University, Nanjing 210093, China
$^7$Diamond Light Source, Harwell Science and Innovation Campus, Didcot OX11 0DE, United Kingdom

(Received 29 August 2015; revised manuscript received 17 December 2015; published 11 January 2016)

We report an angle-resolved photoemission spectroscopy study of a ThCr$_2$Si$_2$-type superconductor YFe$_2$Ge$_2$ ($T_c \approx 1.8$ K) in the normal state. The resolved low-energy band structure mainly consists of several flat Fe bands, while the renormalization factors of different bands range from 1.7 to 2.8. Around the Fermi level, these bands contribute to a high density of states, which may account for the unusually high Sommerfeld coefficient $\gamma$. Besides, a 30 meV kink is observed, which is probably induced by electron-phonon interactions. Our results indicate that YFe$_2$Ge$_2$ is a moderately correlated compound, while electron-phonon coupling should be taken into account to better understand its properties.

DOI: 10.1103/PhysRevB.93.024506

I. INTRODUCTION

The recent discovery of superconductivity in YFe$_2$Ge$_2$ ($T_c \approx 1.8$ K) has stimulated many research interests [1–6]. Similar to the 122 family of iron-based superconductors, YFe$_2$Ge$_2$ crystallizes in a ThCr$_2$Si$_2$ structure ([4/mmm] [Fig. 1(a)], in which FeGe layers are stacked along the $c$ axis with alternating layers of yttrium ions. On the other hand, the isostructural compound LuFe$_2$Ge$_2$ exhibits antiferromagnetic spin density wave order below 9 K. Through partially substituting lutetium by yttrium, the transition is continuously suppressed, with the magnetic quantum critical point (QCP) lying near a critical composition of Lu$_{0.8}$Y$_{0.2}$Fe$_2$Ge$_2$ [7]. For YFe$_2$Ge$_2$, evidence of fluctuating spin moments on the iron sites has been found in the core level photoemission spectroscopy experiment [2]. First-principles calculations further predicted that there exist competing magnetic interactions in this compound [5]. In this context, several possible superconducting pairing mechanisms have been proposed, including sign-changing $s_\pm$ wave singlet pairing [5] and spin fluctuation mediated triplet pairing [6]. Moreover, the Sommerfeld coefficient of YFe$_2$Ge$_2$ reaches an unusually high value ($\sim$100 mJ/mol K$^2$) for a $d$-electron compound [1,3], which makes YFe$_2$Ge$_2$ even more intriguing.

To reach a better understanding of YFe$_2$Ge$_2$, a comprehensive study of its electronic structure is a prerequisite. In this paper, we report an angle-resolved photoemission spectroscopy (ARPES) study of YFe$_2$Ge$_2$ in the normal state. The observed low-energy band structure is mainly contributed by five Fe bands, three of which intersect the Fermi level ($E_F$), forming two hole pockets around the zone center and one electron pocket around the zone corner. The renormalization factors of different bands are around 1.7–2.8, indicating that electronic correlations are moderate in this compound. Around $E_F$, these bands contribute to a high density of states, which may account for the unusually high Sommerfeld coefficient $\gamma$. Furthermore, we find a kink around 30 meV in the band dispersion, which may be attributed to strong electron-phonon interactions. Our results put constraints on theory and lay the foundation for further investigations of this compound.

II. SAMPLE PROPERTIES AND EXPERIMENTAL SETUP

High quality YFe$_2$Ge$_2$ single crystals were synthesized from tin flux, as described elsewhere [8]. For as-grown crystals, the electron probe microanalysis gives an average composition of Y:Fe:Ge $\approx$ 1:0.0:2.115:1.920. Figure 1(b) presents the x-ray diffraction (XRD) pattern. The narrow peak width in the rocking scan curve guarantees the high crystalline quality of the single crystal [inset of Fig. 1(b)]. YFe$_2$Ge$_2$ is metallic over a wide temperature range (2.5–300 K) and the resistivity data show that the residual resistivity ratio $\rho(300 K)/\rho(2.5 K)$ is typically about 37 [Fig. 1(c)]. The superconductivity in YFe$_2$Ge$_2$ is rather sensitive to the sample quality [3,4]. For our samples, a sharp superconducting transition (around 1.8 K) is only observed in powder [inset of Fig. 1(c)]. In Fig. 1(d), the specific heat data are plotted in the form of $C_p/T$ vs $T^2$. By fitting the low temperature data (6–11 K) with the formula $C_p/T = \gamma + \beta T^2 + \alpha T^4$, the Sommerfeld coefficient $\gamma$ is extrapolated to be 96 mJ/mol K$^2$, while $\beta$ is approximately $2.95 \times 10^{-2}$ mJ/mol K$^4$.

ARPES measurements were performed at Beamline I05-ARPCS of the Diamond Light Source in which a VG-Scienta
R4000 electron analyzer is equipped. The typical angular resolution is 0.2° and the overall energy resolution is better than 20 meV for the photon energies used. Samples were cleaved in situ and measured under an ultrahigh vacuum of better than 8 × 10^{−11} Torr.

III. EXPERIMENTAL RESULTS

The three-dimensional Brillouin zone (BZ) of YFe2Ge2 is illustrated in Fig. 2(a). To determine the correspondence between the typical photon energies and the high-symmetry points, we plot the energy distribution curves (EDCs) recorded at normal emission as a function of photon energy [Fig. 2(b)]. A wide range of photon energies is used here to cover more than one whole BZ along the k,c direction. A periodic variation of the peak positions for the band around −400 meV can be observed. Using the free electron final-state model [9] with an inner potential of 12 eV, we estimate 80 eV for the ΓXM plane, and 62/101 eV for the ZRA plane.

Next, we examine the low-lying band structure of YFe2Ge2 along high-symmetry directions. The photoemission intensity plots taken around the ZRA plane are presented in Figs. 3(a) and 3(d). Along Z-A, by tracking the peaks in the corresponding EDCs around the zone center [Fig. 3(b)], two bands assigned as α and γ can be resolved around −20 and −400 meV, respectively. From the momentum distribution curves (MDCs) near EF, one hololike band can be distinguished to cross EF [Fig. 3(c)]. It further disperses backwards to EF around the zone corner [Fig. 3(b)], and we...
FIG. 4. The photoemission data taken around the Γ point. (a) The photoemission intensity plot taken with 80 eV circularly polarized photons along the Γ-M direction. (b) The corresponding EDCs for the data in (a). (c) The corresponding MDCs for the data in (a). (d)–(f) The same as those in (a)–(c), but taken along the Γ-X direction. Dashed lines are guides for the eye for band dispersions. Data were taken at 7 K.

assign this band as β. Around the A point, we can find one more hololelike band with a larger Fermi crossing and an electronlike band from the corresponding EDCs and MDCs [Figs. 3(b) and 3(c)]. These two bands are assigned as δ and η, respectively. Along Z-R, β and δ cross $E_F$, forming two hole pockets, while α sinks below $E_F$ [Figs. 3(d)–3(f)]. Thus, as depicted in Fig. 2(c), the resulting Fermi surface consists of one circular hole pocket, one rounded rectangle hole pocket around the zone center, and one elliptical electron pocket around the zone corner. The strong intensity at the zone center corresponds to the residual spectral weight of α, which leads to some additional peaks around $E_F$ in the corresponding MDCs as well [Figs. 3(c) and 3(f)].

In Fig. 4, we present the photoemission data taken around the ΓX plane. The detailed EDCs and MDCs are shown in Figs. 4(b), 4(c), 4(e), and 4(f), respectively. Except for an intensity variation of some bands, the band structure observed here roughly coincides with that around the ZRA plane. Especially, the band dispersions along Γ-X are almost identical to those along Z-R [Figs. 3(d) and 4(d)]. In Figs. 5(a) and 5(b), we present the photon-energy dependence of the MDCs integrated along Γ(Z)-X(R) and the EDCs at the M(A) point. Only a weak variation of the peak positions upon varying the photon energies is observed, indicating that the electronic structure is quasi-two-dimensional. Here, we emphasize that our measured data do not originate from surface states since surface states should be purely two dimensional and no periodicity of the band(s) upon changing photon energy could be found. However, according to the calculations [5,6], the electronic structure of YFe2Ge2 is highly three dimensional. In Fig. 5(c), we present the band calculations along the high-symmetry directions, showing the highly three-dimensional nature of the band structure. The corresponding band structure along high-symmetry directions. Along XΓM, solid lines are guides to the eye for the band dispersions. Along RZA, the calculated band dispersions are renormalized by a factor of 2.5 and overlaid on the photoemission intensity plot for comparison.
of the electron momentum component perpendicular to the sample surface \( \delta k_z = 1/\lambda \sim 0.2 \, \text{Å}^{-1} \), which is about 16% of the length of the BZ \((4\pi/c \sim 4 \times 3.14/10.42 = 1.2 \, \text{Å}^{-1})\). We note that such broadening may not be sufficient to account for the situation observed here. Other broadening effects or the validity of the band calculations are yet to be explored.

It is worth noting that a kinklike feature is observed in the dispersion of the \( \delta \) band along \( \Gamma(Z)-X(R) \) [Fig. 6(a)], which is a typical manifestation of strong electron-phonon coupling. This kink is observed across the whole BZ along \( k_z \). We select the data in three typical \( k_z \) planes, the \( ZRA \) plane (101 eV), the \( \Gamma X M \) plane (80 eV), and an intermediate \( k_z \) plane (89 eV) as representatives for the analyses below.

We extract the dispersion of \( \delta \) from the corresponding MDCs [as exemplified in Fig. 6(b)]. The high-energy dispersion is fitted linearly and used as an approximation of the bare band dispersion without an electron-phonon interaction [11,12]. The kink is located at around 30 meV [Fig. 6(b)], which coincides with the Debye temperature extrapolated from our transport analysis of the kink structure.

FIG. 6. The analysis of the kink. (a) The magnified photoemission intensity plot around the kink taken with circularly polarized 101, 89, and 80 eV photons, respectively. (b) The dispersion of the \( \delta \) band (89 eV) obtained by fitting the corresponding MDCs. The red dashed line is obtained by fitting the high-energy dispersion linearly. The blue thick line roughly indicates the mode energy. (c), (d) The self-energy analysis of the kink structure.

The high-energy dispersion is approximated by the full width at half maximum of the Lorenzian peaks used to fit the MDCs [Fig. 6(d)]. Around 30 meV, there are clear peaks in the Re \( \Sigma(\omega) \) and rapid decreases in the \( |2 \, \text{Im} \, \Sigma(\omega)| \) for all the representative \( k_z \)'s, as expected in the presence of electron-phonon coupling. Based on the gradient of the experimental Re \( \Sigma(\omega) \) near \( E_F \), the coupling parameter can be estimated to be \( \lambda = 1.19 \pm 0.14 \) (101 eV), 1.03 \( \pm \) 0.10 (89 eV), and 0.94 \( \pm \) 0.11 (80 eV), respectively. The enhancement of the FWHM of the Lorenzian peaks is due to the electron correlations resembling those observed in pnictides [13,14]. The large background may be attributed to the inelastic scattering induced by impurity or the nearness to a magnetic QCP.

Here, we note that the kink is only clearly observed in the \( \delta \) band. However, we cannot exclude the possibility of kinklike features in other bands’ dispersion. For YFe\(_2\)Ge\(_2\), except for the \( \delta \) band, other bands in the vicinity of \( E_F \) are all rather flat, which may hinder the observation of a kink. Furthermore, the proximity of these bands makes it challenging to determine precisely the band dispersions.

IV. DISCUSSION AND CONCLUSION

To obtain the information of the electronic correlation strength of YFe\(_2\)Ge\(_2\), we renormalize the bands given by calculations to fit those observed by ARPES and summarize the results in Fig. 5(d). Quantitatively, around the \( \Gamma XM \) plane, the renormalization factors for different bands are around 1.7–2.1, while around the \( ZRA \) plane, the overall renormalization factors are about 2.4–2.8. For comparison, the renormalization factor of BaFe\(_2\)As\(_2\) is around 2–3 [15–17]. From an ionic picture, the Fe electron occupation (given by calculations) in YFe\(_2\)Ge\(_2\) is 3\( d^{0.5} \) [5]. The larger occupation number of electrons than that in BaFe\(_2\)As\(_2\) (3\( d^6 \)) weakens the Hund’s interaction, leading to reduced electron correlations. Moreover, the Fe-Ge bond length (2.393 Å) is found to be smaller than the Fe-As bond length (2.403 Å), which favors electron hopping. The above qualitative analysis suggests that the overall correlation strength of YFe\(_2\)Ge\(_2\) should be weaker than that of BaFe\(_2\)As\(_2\). Consistently, for materials with a higher electron occupation, for instance, BaNi\(_2\)As\(_2\) (3\( d^8 \)) and KNi\(_2\)Se\(_2\) (3\( d^{8.5} \)), the renormalization factors monotonically decrease to 1.66 and 1.54, respectively [18,19].

This moderate electron correlation of YFe\(_2\)Ge\(_2\) seems to be in contradiction to its high Sommerfeld coefficient. Such behavior has also been reported in TlNi\(_2\)Se\(_2\) and KNi\(_2\)Se\(_2\) [19,20], which has been explained by a rather large density of states at \( E_F \). Following the same procedure described in Ref. [19], we use our photoemission data to estimate the \( \gamma \) coefficient by the formula \( \gamma \propto \sum_n \int_{kF} \frac{ds}{n^2 |\Delta k|^2} \), in which \( n \) is the band index, \( ds \) is the perimeter of the Fermi surface, and \( |\Delta k| \) is the Fermi velocity at \( E_F \). We use the 104 eV data in which the band structure is better defined and simplify the estimation by regarding the system as a quasi-two-dimensional one. The obtained \( \gamma \) is about 22.2 eV\(^{-1} \) Å\(^{-2} \). Through interpolation [19], the \( \gamma \) is extracted to be roughly 67 mJ/mol K\(^2\), which is in rough agreement with the one obtained in the specific heat measurement (96 mJ/mol K\(^2\)). This indicates that the large Sommerfeld coefficient should be attributed to the high density of states at \( E_F \) as well. The underestimation of \( \gamma \) by our photoemission data might be caused by the following reasons.

First, due to the overwhelming intensity of \( \alpha \), we may miss the extra Fermi surface contributed by \( \delta \) around the zone center [Fig. 5(d)], which may also contribute a sizable density of states at \( E_F \). Second, although \( \alpha \) sinks below \( E_F \), its broad linewidth of EDCs suggests that there exists a certain amount...
of states at $E_F$, which we have not taken into account in our simplified estimation.

Recent neutron scattering experiments detected two coexisting magnetic fluctuations in YFe$_2$Ge$_2$ at low temperatures [21], namely, $A$-type and stripe antiferromagnetic fluctuations, providing evidence that the superconductivity may be mediated by spin fluctuations. However, with a sizable density of states at $E_F$, the speculation that the superconductivity is mediated by an electron-phonon interaction also makes sense. In this regard, YFe$_2$Ge$_2$ resembles 2H-NbSe$_2$ (a conventional superconductor with $T_c = 7.2$ K) in the sense that they share a similar electron-phonon coupling strength and mode energy [22]. Further investigations are required to distinguish these different scenarios.

To summarize, we report an ARPES study of YFe$_2$Ge$_2$ in the normal state. The electronic correlations are moderate in this compound. Moreover, we find a 30 meV boson mode in the band structure, which is most probably caused by electron-phonon coupling. Our results put constraints on theory and lay the foundation for further investigations of this compound.

ACKNOWLEDGMENTS

We thank the Diamond Light Source for access to Beamline I05-ARPES (Proposal No. SI10213) that contributed to the results presented here. This work is supported in part by the National Science Foundation of China and National Basic Research Program of China (973 Program) under Grants No. 2012CB921402, No. 2012CB927401, No. 11274332, and No. 11272902. D.W.S. is also supported by the “Strategic Priority Research Program (B)” of the Chinese Academy of Sciences (Grant No. XDB04040300).