BL-28A/2012G771

Electronic structure of $K_{1.08}Ni_{2.01}Se_{1.92}$ studied by angle-resolved photoemission spectroscopy

Qin Fan[1*], Zirong Ye[1], Min Xu[1] and Donglai Feng[1]
[1]State Key Laboratory of Surface Physics, Department of Physics,
and Advanced Materials Laboratory, Fudan University, Shanghai 200433, People's Republic of China

1 Introduction

The discovery of iron-based superconductors with the superconducting transition temperature up to 55K in iron pnictides has generated great interests [1,2]. However, the sibling Ni-based compounds only possess relatively low transition temperature. It is intriguing to figure out why T_c is low in the Ni-based compounds, which may facilitate understanding the high-T_c superconductivity in iron-based ones. Recently the newly discovered KNi_2Se_2 superconductor was found to exhibit several remarkable physical properties. At high temperatures, the material has high resistivity and constant magnetic susceptibility, indicating Pauli paramagnetic response. Structural analysis reveals that the material has at least three distinct subpopulations of Ni-Ni bond lengths. At temperature below 20 K, the structural distortions disappear, and the material enters a coherent heavy-fermion-like state with effective electron mass $m^* \sim 10m_e$. When cooling down to 1K, superconductivity emerges. [3-5].

2 Experiment

Single crystals of $K_{1.08}Ni_{2.01}Se_{1.92}$ were grown by self-flux method with nominal composition K:Ni:Se = 1.02:2:2. Prereacted NiSe and K pieces were added together into the alumina crucible and then sealed in a Fe crucible. They were heated to 1000 ℃, kept at this temperature for 3 hours, then cooled to 600 ℃ with 4 ℃/h. The dark pink single crystal is sensitive to the air. All the preparation work must be done in Ar-filled glove box.

With the high performance of Beamline 28A in Photon Factory, we have systematically studied the electronic structure of KNi_2Se_2. High-quality data were collected. By changing the tilt, we could map out the Fermi surface of KNi_2Se_2. By further conducting photon energy dependent measurements, we could obtain the Fermi surface topology in three-dimentional (3D) Brillouin zone.

3 Results

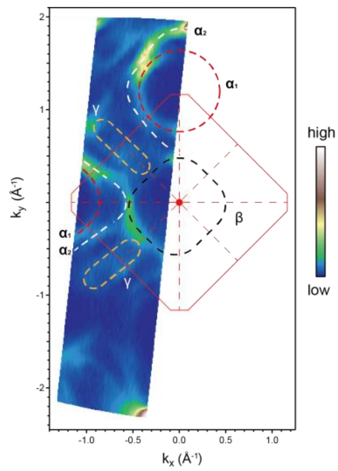

Fig. 1: Photoemission intensity distribution integrated over [E_F-10 meV, E_F+10 meV] window for $K_{1.08}Ni_{2.01}Se_{1.92}$ taken at 60K with 75 eV photons in circular experimental geometry.

The photoemission intensity maps of $K_{1.08}Ni_{2.01}Se_{1.92}$ at the Fermi energy is displayed in Fig.1. The data of Fig.1 were taken with 75eV photons in the circular experimental geometry. The Fermi surface is consisted of electron pockets. The Fermi crossings are determined and four main features are labeled as $\alpha_{1,2}$, β, γ. According to our results, $\alpha_{1,2}$ are the electron pockets surrounding zone corner. β represents the pocket around zone center. While, γ corresponds to another slim ellipse electron pocket around X. This agrees with that $K_{1.08}Ni_{2.01}Se_{1.92}$ is an electron-doped material.

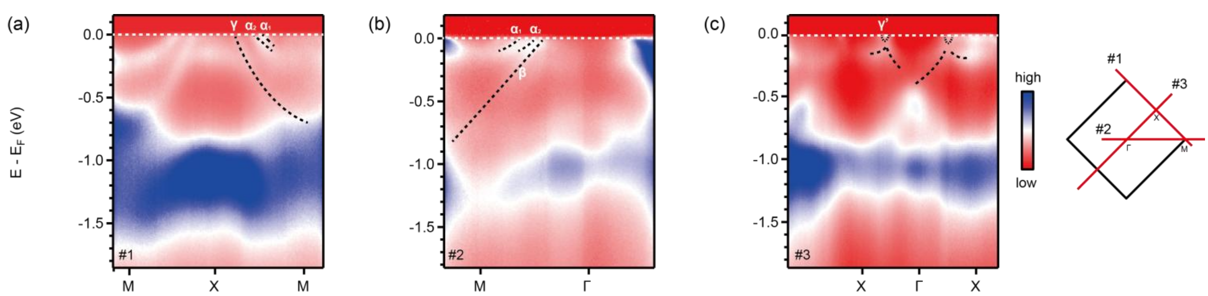

Fig. 2: (a)-(c) Photoemission data along the M-X, Γ-M, Γ-X direction taken with 75eV photons in circular polarization geometry at 60K.

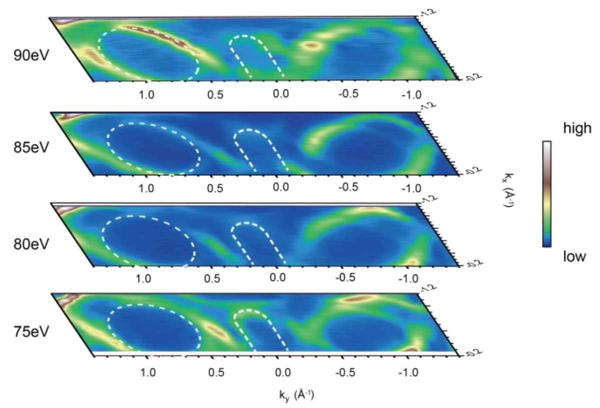

Fig. 3: Fermi surface taken with 75eV, 80eV, 85eV and 90eV photons, respectively at 60K.

Now we turn to the low-lying band structures. The data were taken with 75eV photon energy in circular light at 60K. Taking the inner potential of 13eV, 75eV corresponds to the Γ point. Fig. 2 shows the photoemission intensity taken along high-symmetry directions. In the M-X direction, three electron-like bands, named α_1, α_2 and γ, are observed. The $\alpha_{1,2}$ bands are close to each other at the Fermi energy. In the Γ-M direction, besides α_1, α_2 bands, another band named β is resolved. In the Γ-X direction, there is another small electron-like band named γ' as illustrated in Fig. 2(c). The $\alpha_{1,2}$, β and γ band are attributed to the electron pockets surrounding M, Γ and X, respectively. β and γ look like hole-like bands, actually they are electron-like bands around M. The band bottoms of $\alpha_{1,2}$, β and γ approach ~0.2eV, ~0.9eV, and ~0.7eV below Fermi energy, respectively.

The observed band structure also agrees well with the theoretical calculation which is reported by Feng Lu et al. The renormalization factor Z is ~ 1.8, indicating that this material is a weak correlation system. [6]

To determine the Fermi surface topology in the 3D momentum space, through changing the photon energy, we have mapped out the Fermi surface as shown in Fig. 3. The data in figure 3 is taken at 60K and with 75eV, 80eV, 85eV, 90eV photons, respectively. It is shown that the Fermi surface is almost unchanged with the photon energy, indicating the 2D character of the KNi_2Se_2 system.

<u>References</u>

[1] Y.Kamihara et al., J.Am.Chem.Soc. 130,3296(2008).
[2] X.H.Chen et al., Nature(London) 453,761(2008).
[3] J.R.Neilson et al., Phys.Rev.B 86, 054512 (2012).
[4] H.C.Lei et al., http://arxiv.org/abs/1211.1371(2012).
[5] J.R.Neilson et al., J.Am.Chem.Soc. 134, 7750 (2012).
[6] F.Lu et al., J.Phys.:Condens.Matter 24,495501 (2012).

* 11110190010@fudan.edu.cn