X-ray Compton scattering reveals electronic motions with a preferred direction in high-temperature cuprate superconductors

An X-ray can be scattered by electrons and lose energy. This process is called X-ray Compton scattering. The scattered X-ray carries information about the momentum distribution $n(\mathbf{k})$ of electrons. In metals, $n(\mathbf{k})$ exhibits a rapid change at the Fermi momentum $\mathbf{k}_F$, above (below) which electron occupation becomes low (high). The surface corresponding to $\mathbf{k}_F$ is called the Fermi surface (FS), the shape of which reflects electron motions inside the metal. The FS is recognized as a fundamental concept in understanding material properties.

High-temperature cuprate superconductors continue to be a central subject in condensed matter physics [1]. They are characterized by a stack of CuO_2 planes, and a vast number of studies using angle-resolved photoemission spectroscopy (ARPES) have confirmed the existence of the two-dimensional (2D) FS at least in the overdoped region — the critical temperature T_c in cuprate superconductors is controlled by the carrier doping rate. In the underdoped region including the optimal doping at which T_c becomes maximal, the FS was observed clearly only around $\mathbf{k}$ = (0.45π, 0.45π) — the so-called Fermi arcs, which were believed to be a portion of the underlying 2D FS [2].

To reveal the underlying FS, we perform Compton scattering for the La-based cuprate $La_{2-x}Sr_xCuO_4$ with $x = 0.08$ (underdoped sample) at SPring-8 **BL08W** [3]. The obtained momentum distribution $n(\mathbf{k})$ is shown in Fig. 1 in the first Brillouin zone $-\pi < k_x,\ k_y < \pi$. Is Fig. 1 consistent with the conventional 2D FS illustrated in Figs. 2(a) and 2(b)? There are two key criteria: $n(\mathbf{k})$ should be nearly constant along the FS and the derivative of $n(\mathbf{k})$, i.e., $\nabla n(\mathbf{k})$, increases in magnitude there.

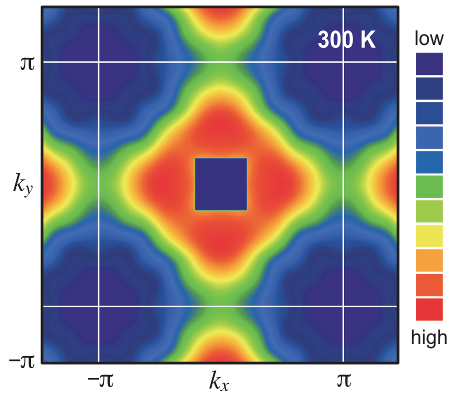

Fig. 1. Electron momentum distribution measured by Compton scattering at 300 K for $La_{2-x}Sr_xCuO_4$ with $x = 0.08$ [3]. Red (blue) indicates a higher (lower) occupation of electrons. Data around $\mathbf{k} = (0,0)$ are removed because of low accuracy. [5]

In Fig. 2(c), we superpose the FS identified by ARPES (dots) [2] by focusing on the first quadrant of the Brillouin zone. Around $\mathbf{k}$ = (0.45π, 0.45π), $n(\mathbf{k})$ is nearly constant along the FS as expected. However, around $\mathbf{k}$ = (π, 0) and (0, π), $n(\mathbf{k})$ varies along the FS (from yellow to green), implying that the underlying

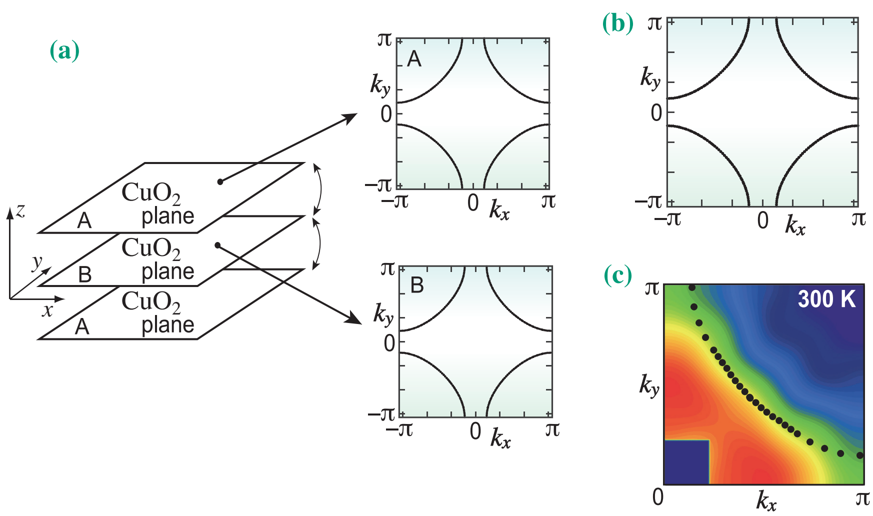

Fig. 2. Conventional idea. **(a)** 2D-like FS is realized in each CuO_2 plane. **(b)** Bulk FS. **(c)** Observed $n(\mathbf{k})$ in the first quadrant of the Brillouin zone. The FS identified by ARPES (dots) is superposed. [5]

FS cannot be the conventional one accepted thus far (Figs. 2(a) and 2(b)). We also examined the data of $\nabla n(\mathbf{k})$, which indicated a curvature qualitatively different from that of the conventional FS [3].

The agreement between the results of the present work and ARPES around $\mathbf{k} = (0.45\pi, 0.45\pi)$ is reasonable because ARPES signals are very clear there. However, the signals become weak and broad upon approaching $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$, which makes it difficult to identify the FS. Hence, the underlying FS was inferred by extrapolating the FS observed clearly around $\mathbf{k} = (0.45\pi, 0.45\pi)$ to a region around $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$, as shown by dots in Fig. 2(c) [2]. However, such a FS cannot be reconciled with our data, especially around $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$.

What does Compton scattering data Fig. 1 then imply? One possibility is an electronic nematic tendency — the electron motion has a preferred direction along the *x*- or *y*-direction in each CuO_2 plane; this tendency is enhanced in the underdoped region in cuprates [4]. For La-based cuprates, this theory [4] predicted that the electronic nematicity yields a quasi-one-dimensional FS in each CuO_2 plane and the direction of nematicity alternates along the *z*-direction through a coupling to the crystal structure; see Fig. 3(a). These FSs are hybridized via weak interlayer coupling, leading to 2D-like FSs, consisting of the inner and outer FS as shown in Fig. 3(b).

We superpose those FSs on the observed $n(\mathbf{k})$ in Fig. 3(c). The inner FS explains $n(\mathbf{k})$, which is essentially constant (yellow) along the FS. Similarly, the outer FS may also explain $n(\mathbf{k})$, although $n(\mathbf{k})$ changes along the FS around $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$ from green to blue. We observed that the value of $\nabla n(\mathbf{k})$ is very small there and thus the actual change in $n(\mathbf{k})$ can be considered to be not sizable. We also performed the same analysis of data at 150 K and confirmed this conclusion. Upon reaching the overdoped region, it is expected that the FS in Fig. 3(a) will lose nematicity and become conventional 2D FS [4]. This expectation was also confirmed by performing Compton scattering at $x = 0.15$ and 0.30 [3].

In summary, X-ray Compton scattering reveals that, in contrast to the common belief (Fig. 2), electrons in La-based cuprates have a preferred direction along the *x*- or *y*-direction in each CuO_2 plane and the preferred direction alternates between the layers (Fig. 3). Compton scattering can be a powerful tool, especially when other probes such as ARPES cannot reveal the whole shape of the FS.

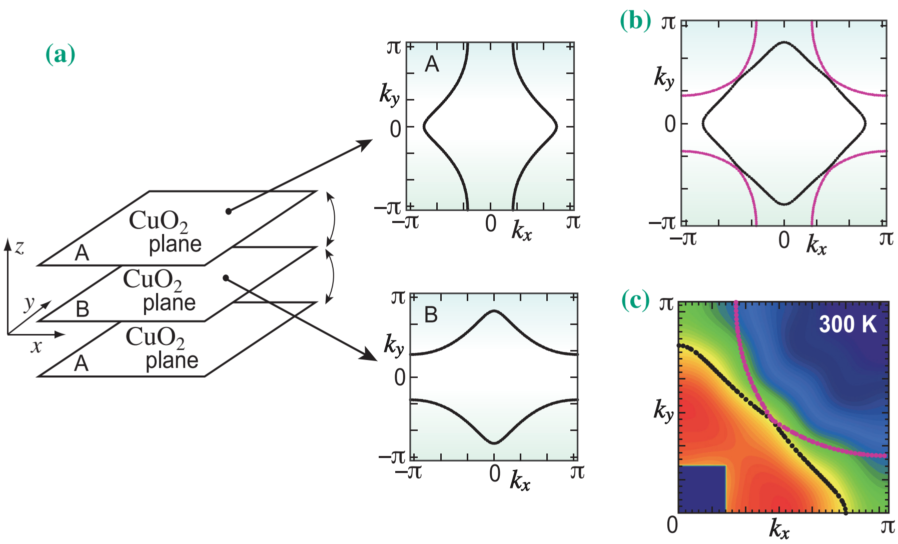

Fig. 3. Electronic nematic scenario. **(a)** FS stacking where the preferred direction of the electron motion is rotated 90 degrees between adjacent layers. **(b)** Bulk FSs consist of the inner (black) and outer (purple) FSs. **(c)** Observed $n(\mathbf{k})$ in the first quadrant of the Brillouin zone. The FS in (b) is superposed. [5]

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References

[1] B. Keimer *et al.*: Nature **518** (2015) 179.
[2] T. Yoshida *et al.*: J. Phys. Soc. Jpn. **81** (2012) 011006.
[3] *H. Yamase, Y. Sakurai, M. Fujita, S. Wakimoto and K. Yamada: Nat. Commun.* ***12*** *(2021) 2223.*
[4] H. Yamase and H. Kohno: J. Phys. Soc. Jpn. **69** (2000) 332; *ibid.* 2151.
[5] H. Yamaes and Y. Sakurai: Isotope News **779** (2022) 38.