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Article

Temperature-induced Lifshitz transition in topological insulator candidate $HfTe_5$

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ABSTRACT

The ongoing discoveries and studies of novel topological quantum materials have become an emergent and important field of condensed matter physics. Recently, $HfTe_5$ ignited renewed interest as a candidate of a novel topological material. The single-layer $HfTe_5$ is predicted to be a two-dimensional large band gap topological insulator and can be stacked into a bulk that may host a temperature-driven topological phase transition. Historically, $HfTe_5$ attracted considerable interest for its anomalous transport properties characterized by a peculiar resistivity peak accompanied by a sign reversal carrier type. The origin of the transport anomaly remains under a hot debate. Here we report the first high-resolution laser-based angle-resolved photoemission measurements on the temperature-dependent electronic structure in $HfTe_5$. Our results indicated that a temperature-induced Lifshitz transition occurs in $HfTe_5$, which provides a natural understanding on the origin of the transport anomaly in $HfTe_5$. In addition, our observations suggest that $HfTe_5$ is a weak topological insulator that is located at the phase boundary between weak and strong topological insulators at very low temperature.

1. Introduction

The topological quantum materials, representing a new state of condensed matter, have attracted remarkable interest in recent years. Many of them have been predicted in theory and realized in experiment, including three-dimensional or two-dimensional topological insulators [1–7], three-dimensional Dirac semimetals [8–18] and three-dimensional Weyl semimetals [19–28], nodal line semimetals [29,30] and latest "new Fermion" topological materials [31,32]. These materials exhibit rich physics and promising prospect for applications in future electronics and spintronics. Furthermore, the topological phase transition between these topological states of matter is new and distinct from the traditional Landau phase transition. Very recently, the transition-metal pentatellurides, $HfTe_5$ or $ZrTe_5$, have ignited renewed interest as a candidate of a novel topological material [33]. The single-layer $HfTe_5$ and $ZrTe_5$ are predicted to be two-dimensional large band gap topological insulators (or quantum spin Hall insulator); a topological phase transition is expected in bulk materials that can be driven even by temperature [33]. Historically, $HfTe_5$ and $ZrTe_5$ are well-known thermoelectric materials. They exhibit unusual transport properties characterized by a strong resistivity peak [34–36] accompanied by a sign reversal of the Hall coefficient and thermopower across the peak temperature [37–39]. The origin of the transport anomaly is still controversial [36,39–43].

In exploring the topological nature and addressing the origin of the transport anomaly in $ZrTe_5$, many recent experiments conclude its bulk as either a topological insulator [44–48], or a three-dimensional Dirac semimetal [49–52], or a quasi-two dimensional Dirac semimetal [53,54], or two/three dimensional massive Dirac fermion system [55,56]. For $HfTe_5$, the theoretically predicted topological properties have rarely been studied experimentally, and recent transport experiments point to its being a three-dimensional topological insulator at low temperature [57,58]. Up to now, a unified understanding of the topological nature in $ZrTe_5$

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and $HfTe_5$ is still lacking. The electronic structure study of $HfTe_5$ is highly anticipated.

In this paper, we report the first electronic structure study on $HfTe_5$ by high resolution laser-based angle-resolved photoemission spectroscopy (ARPES) measurements. Regarding the overall electronic structure and its temperature evolution, we find that $HfTe_5$ behaves quite similarly to that of $ZrTe_5$ [48]. The transport properties of $HfTe_5$ is dominated by two branches of fast dispersive energy bands, a valence band and a conduction band, at the Brillouin zone center. With decreasing temperature, these two bands gradually shift downward and come closer to each other, but with a gap between them that persists down to 15 K. This gives rise to an intriguing electronic structure evolution in $HfTe_5$ from a p-type-semimetal at high temperature above ~65 K, to a semiconductor at the resistivity peak temperature ~65 K, and to an n-type semimetal at low temperature. These results indicate a temperature-induced Lifshitz transition in $HfTe_5$. It provides a natural understanding on the transport anomaly at ~65 K. The quantitative difference of transport properties between $HfTe_5$ and $ZrTe_5$ are reflected in the subtle difference of their electronic structures. Based on the detailed comparison between the electronic structures we measured on $ZrTe_5$ in Ref. [48] and $HfTe_5$ in this work, we will also discuss the topological nature of $HfTe_5$ and $ZrTe_5$.

2. Experimental

High quality single crystal samples of $HfTe_5$ and $ZrTe_5$ were grown by the chemical vapor transport method with iodine as transport agent. The ARPES measurements were performed using our new laser-based system equipped with a 6.994 eV vacuum-ultra-violet (VUV) laser and a time-of-flight electron energy analyzer (ARToF10K by Scienta Omicron) which enables us to efficiently collect two-dimensional momentum space photoemission spectra (E_k Vs (k_x, k_y)) simultaneously. The overall energy resolution was set at 1–5 meV, and the angular resolution was 0.1°. All the samples were cleaved *in situ* and measured in ultrahigh vacuum with a base pressure better than 5×10^{-11} mbar (1 mbar = 100 Pa).

3. Results and discussions

As shown in Fig. 1a, $HfTe_5$ is a layered compound that crystallizes in orthorhombic crystal structure similar to $ZrTe_5$ [48]. The bulk $HfTe_5$ is constructed by stacking two-dimensional (2D) $HfTe_5$ sheets along the *b* axis via a weak van der Waals bonding. The 2D $HfTe_5$ sheet is formed by linking the adjacent corrugated prismatic $HfTe_6$ chains via zigzag chains of Te_2 atoms along the *c* axis. The $HfTe_6$ chains run along the *a* axis with a quasi-one-dimensional nature. Thus, the natural cleavage of $HfTe_5$ leaves a shiny and charge-neutral surface (Fig. 1b) that corresponds to the crystalline *a*-*c* plane. The projected surface Brillouin zone with high symmetry momentum points labelled for $HfTe_5$ is shown in Fig. 1c on top of the experimental Fermi surface mapping results.

The typical Fermi surface and band structure of $HfTe_5$ are shown in Fig. 1c and 1d. Fig. 1c illustrates the constant energy contours of $HfTe_5$ measured at 125 K, which represent the energy-integrated spectral weight distribution at selected binding energies of 0 (at the Fermi level), 150 and 300 meV. The corresponding band structures are shown in Fig. 1d taken along high symmetry momentum cuts Γ-*X* and Γ-*Y* as well as a particular cut Γ-*B*. Here, the *B* point is defined as the momentum position of the band bottom for an extra electronic-like band that is above the Fermi level E_F; it is located along the Brillouin zone boundary *YM* (see also Fig. 2a). With increasing binding energy, except for the very weak spectral weight observed at *B* due to thermal excitation of the Fermi-Dirac distribution, the constant energy contour near Γ evolves gradually from a tiny spot at the Fermi level to a small rectangle and eventually to a strongly warped large rectangle. The observed pockets are all hole-like, consistent with the observation of hole-like bands as seen in Fig. 1d. The Fermi level here seems to just cross the top part of the valence band that is consistent with the hole-carriers-dominated transport at high temperature in $HfTe_5$. Just like the band structures in $ZrTe_5$ [48], these hole-like bands show nearly-linear dispersions over a wide energy range and also exhibit a strong anisotropy of the Fermi velocity; it is higher along high-symmetry directions Γ-*X* and Γ-*Y* but lower along Γ-*B* direction. In the case of $ZrTe_5$, after a detailed lineshape analysis and the slab band calculations, the corresponding hole-like bands at Γ point are found to be composed of an envelope of sub-bands arising from the finite k_z effect of ARPES measurements [48]. It can be reasonably inferred that the observed broadening of bands at Γ in $HfTe_5$ most likely has the same origin as that for $ZrTe_5$. Generally speaking, the overall electronic structure of $HfTe_5$ is quite similar to that for $ZrTe_5$ [48].

The $HfTe_5$ samples we measured show a resistivity peak at about 65 K, a characteristic temperature that is much lower than ~135 K in $ZrTe_5$ as reported in most previous work [35–37, 39–43,53,59–61] and is comparable to ~60 K in another form of $ZrTe_5$ samples [49–51,55,62]. To clarify the origin of the anomalous transport properties and examine on a possible topological phase transition driven by temperature, we have carried out systematic ARPES measurements on $HfTe_5$ at different temperatures.

Fig. 2a, b and c show temperature-dependent band structures of $HfTe_5$ along three representative momentum cuts Γ-*B*, Γ-*X* and Γ-*Y*, respectively. The Fermi-Dirac distribution is properly removed in order to resolve the features and bands, above the Fermi level E_F. The observed bands can be divided into three groups: the first group is the central valence band (CVB) around the Γ point that are hole-like; the second group is the central conduction band (CCB) around Γ point that are electron-like with weak spectral weight; the third group is the side conduction band (SCB) that is electron-like with strong spectral weight around the *B* point (only shown in Fig. 2a). The relatively weak spectral weight of CCBs may be caused by photoemission matrix element effect or strong electron-electron scattering between the Γ and *B* points. It is clear that all these CCB, CVB and SCB bands show a pronounced temperature dependence, exhibiting an overall shift towards high binding energy with decreasing temperature. Specifically, the CVB crosses the Fermi level at high temperature (say 185 K); and it gradually moves down below the Fermi level at low temperature (e.g., 80 K). In the mean time, the CCB is well above the Fermi level at high temperature (its band bottom is ~60 meV above E_F at 185 K as presented in Fig. 2a–c),shifts down with decreasing temperature and appears to touch the Fermi level at very low temperature (for example, at 15 K in Fig. 2a–c). The SCB exhibits a similar shift downwards as CCB with temperature decrease, but it always sits above the Fermi level at all temperatures we have measured (~35 and ~5 meV above the Fermi level at 185 and 15 K, respectively, see Fig. 2a(1), a(9) and e). Although the overall band structure shifts downwards with decreasing temperature, it is not a rigid band shift. With decreasing temperature, the CVB exhibits an obvious shift with decreasing temperature at high temperatures above 80 K, but shows little change at low temperature below 65 K. On the other hand, the CCB and SCB show a shift with decreasing temperature in the entire temperature range.

There is a gap between the CVB and CCB. As seen in Fig. 2 d, such a gap can be easily resolved as a valley near E_F in the energy distribution curves (EDCs) at Γ point at different temperatures. Although the CCB has a weak spectral weight, a clear upturn can be identified in the EDCs that can be used to define the low limit of the CCB conduction bands. Using the same procedure as used