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Surface states in noncentrosymmetric superconductor BiPd

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Abstract. BiPd is a noncentrosymmetric superconductor with Dirac-like surface states on both (010) and (0 $\bar{1}$ 0) faces. The Dirac cone on (010) surface is intense and appears at 0.66 eV binding energy. These states have drawn much attention due to contradictory reports on dimensionality and the momentum of these Dirac fermions. We have studied the properties of these Dirac fermions using varied photon energies and different experimental conditions. The behavior of the Dirac cone is found to be two-dimensional. In addition, we found few more surface states appearing at higher binding energies compared to the Dirac cone.

1. Introduction

Topological insulators host symmetry protected states at the surface of band insulators. Bi₂Se₃ is one of the most studied topological insulators [1-4]. Efforts have been made to find such surface states in superconductors which have significant fundamental and technological interests. BiPd is proposed to be one such example which is a noncentrosymmetric superconductor with superconducting transition temperature of 3.8 K [5,6]. Extensive photoemission studies have shown that single crystalline BiPd harbors interesting surface and bulk electronic structure and the Dirac like surface states appear on both (010) and (0 $\bar{1}$ 0) surfaces [7-11]. Spin-resolved photoemission measurements [8] have confirmed the spin-polarization of the surface states appearing on (010) face. Scanning tunneling spectroscopy study [12] shows presence of surface states above the Fermi level also. It has been found [13] that the surface states appearing below the Fermi level are located at \bar{S} , while those appearing above the Fermi level are located at \bar{F} (see figure 1(a)). The Dirac like surface states on (010) surface lie at 0.66 eV binding energy and are imaged clearly in ARPES experiments. But the states on (0 $\bar{1}$ 0) surface lie near the Fermi level in the vicinity of the bulk states and are not resolved properly in ARPES experiments. Because of twinning in the BiPd single crystals, simultaneous ARPES imaging of both (010) and



($0\bar{1}0$) surfaces is possible [10]. At the same time it becomes difficult to tell on which face a particular surface state resides.

The Dirac like states which appear at 0.66 eV binding energy on (010) face have drawn much attention due to conflicting reports about its properties. Both dimensionality and momentum of these bands are under scrutiny. While density functional theoretic calculations conclude it to be two-dimensional, photon energy dependent ARPES [9] shows its possible three-dimensional nature. Also, few studies report the Dirac point to be located at the centre of the surface Brillouin zone $\bar{\Gamma}$ [8,9], while others report it to be at the edge of the surface Brillouin zone \bar{S} (see figure1(a)) [10,13]. In this work [11], we have shown photon energy dependent results, which are consistent with the two-dimensional nature of the Dirac band. Apart from this Dirac state, we have discovered few more surface states.

2. Experimental Details

Single crystals of BiPd were prepared using modified Bridgman method by Joshi *et al.* [5]. Good crystallinity was ensured by Laue diffraction method. Samples were cleaved inside the vacuum chamber along the b axis for ARPES measurements. ARPES were carried out in I05 beamline, Diamond light Source, UK and VUV beamline, Elettra, Italy. Total energy resolutions in the Diamond light source and Elettra were 5 meV and 10 meV, respectively.

3. Results and Discussions

To find the momentum and dimensionality of the Dirac bands, experiments were performed in two experimental geometries using various photon energies. Sample position was optimized at one photon energy to get a clear image of the Dirac point, i.e. without any energy gap at the Dirac point. But as the photon energy is varied, an energy gap at the Dirac point opens up in both cases. The energy

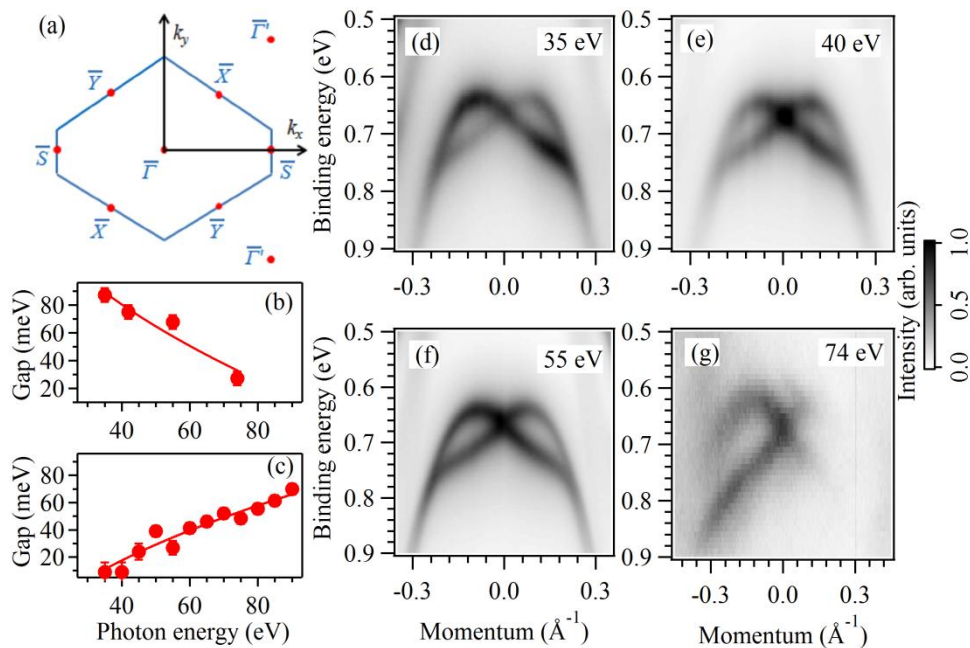


Figure 1. (a) Surface Brillouin zone of BiPd. Energy gap at the Dirac point is shown for two sets of data using the sample position optimized at (b) 74 eV and (c) 35 eV photon energies. Zero energy gap can be obtained by optimizing the sample at each photon energy. Spectra taken along $\bar{\Gamma}$ - \bar{S} - $\bar{\Gamma}$ at (d) 35 eV, (e) 40 eV, (f) 55 eV, and (g) 74 eV photon energies are shown.

gaps at the Dirac point obtained at different photon energies for two sets of measurements are shown in figures 1(b) and (c). The gap shows opposite trends for the two sets. The gradual opening of energy gap with photon energy may indicate a possible three-dimensional character of the Dirac band. It is known that the properties of a three-dimensional band show repetition as the probing photon energy is varied. Because the photon energy is directly linked to the out-of-plane momentum k_z . But our study over a large photon energy range spanning several Brillouin zones shows no periodicity in the gap value which is clear from figure 1(c). Moreover, one can make the gap zero by reoptimizing the sample position at different non-equivalent photon energies.

Opening of energy gap at the Dirac point can also happen due to the sample geometry. Features appearing at $\bar{\Gamma}$ point will remain unchanged even if the photon energy is changed. Finite momentum of the Dirac point will correspond to different emission angle if the photon energy is changed. Thus, the above observations suggest that the position of the Dirac point maybe away from the $\bar{\Gamma}$ -point. By analyzing the angular position of the Dirac point in the spectrum at various energies we found that the Dirac cone on (010) surface is located at \bar{S} [11]. After accounting for the gap arising due to the sample geometry, we get zero-gap condition at each photon energy. Evidently, the bandgap at the Dirac point is not an inherent property of the sample. The sample position can be optimized at different photon energies to image the Dirac point without any energy gap. Figures 1(d)-(g) show the Dirac cone with zero-gap at few photon energies. This supports the two-dimensional nature of the Dirac band.

The dispersion of the Dirac band very quickly deviates from the linear dispersion as is clear from figures 1(d)-(g). Linear energy dispersion is maintained only very close to the Dirac point. It also looks very different from parabolic dispersion. Hence the consideration of the mass term, which is quadratic in momentum, is important; but it also cannot explain the dispersion well. Quadratic mass term and Rashba-like linear term together give rise to a parabolic dispersion. This suggests the importance of higher-order spin-orbit terms in the Hamiltonian of the Dirac states [14,15]. We find that the spin-orbit terms up to third order in momentum can explain all the experimental observations well [11].

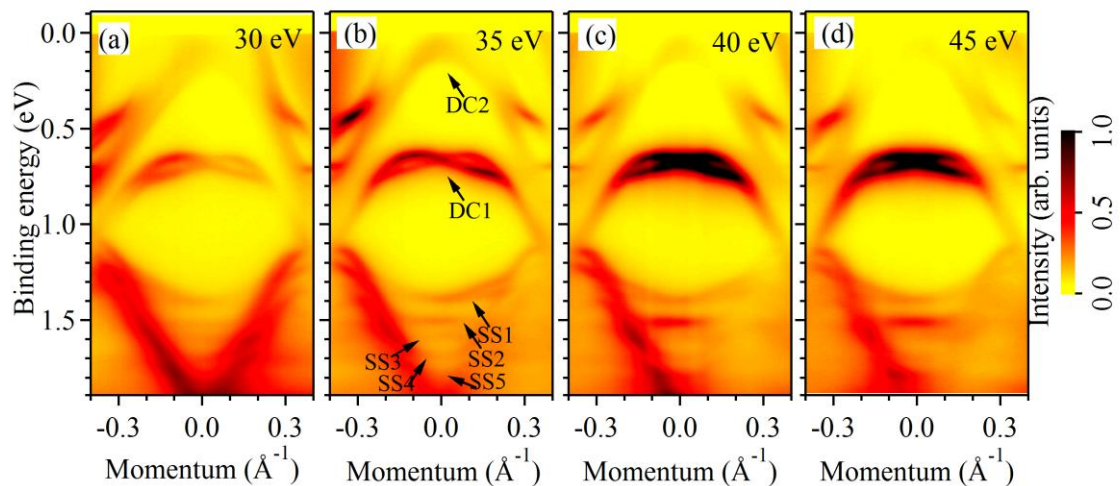


Figure 2. Spectra at (a) 30 eV, (b) 35 eV, (c) 40 eV, and (d) 45 eV. DC1 and DC2 in (b) denote Dirac cones on (010) and (0 $\bar{1}$ 0) surface, respectively. SS1-SS5 denote additional surface states.

Next, we show that apart from the well-known Dirac cone there exist several other surface states in single-crystalline BiPd. Spectra collected at various photon energies are shown in figures 2(a)-(d). In

figure 2(b), DC1 denotes the Dirac cone on (010) surface and DC2 is the Dirac cone on (0 $\bar{1}$ 0) surface. Apart from DC1 and DC2 we see that several other states labeled as SS1-SS5 are present in the spectrum. All of these states are present in the spectrum of every photon energy shown in figure 2. Binding energies of the bands SS1-SS5 do not vary as the photon energy is changed suggesting that they are two-dimensional in nature [11]. Also, these bands are not seen in the bulk band structure calculations. These results suggest that these bands represent the surface states of BiPd.

4. Conclusions

In summary, we have done photon energy-dependent ARPES on BiPd single crystals. The Dirac cone acquired using various photon energies and sample optimizations unambiguously suggest two dimensional behavior of the Dirac fermions and the Dirac point appears at $\bar{5}$. In addition, we discover several other surface bands at higher binding energies. These results suggest coexistence of the Dirac fermions and the normal surface states in this system. The binding energy of the Dirac Fermions is too high to have significant role in the ground state properties of this system.

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