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Pressure Induced Surface States and Wannier Charge Centers in Ytterbium Monoarsenide

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We demonstrate that the XMR material ytterbium monoarsenide (YbAs) shows transitions from a trivial to a non-trivial topological phase with hydrostatic pressure of 20 GPa and maintains its topological character up to structural phase transition pressure. We observed band inversions close to the Fermi level at the X high symmetry point at 20 GPa and band parities are used to confirm the same with consideration of Spin-orbit coupling (SOC) effect. The evolution of the surface states and the bulk band structure in YbAs are discussed.

Keywords: Ytterbium monoarsenide; Topological phase; Fermi level; Spin-orbit coupling

1 Introduction

The Z_2 topological semimetals are a subclass of topological materials. These can be distinguished from trivial insulator via Z_2 topological invariant and requires time-reversal symmetry (TRS) to protect their nontrivial topological characteristics. These topological systems do not exhibit a gap in the bulk band structure *e.g.*, rare earth monopnictide LnPn (Ln = Ce, Pr, Sm, Gd, Yb; Pn = Sb, Bi)[1]. These systems have shown the Z_2 topological character at ambient pressure. However, LaAs[2], LaSb[3],TmSb[4], PbTe, PbS, PbSe, GeTe[5]exhibited inversion when external pressure is applied. Similarly, the rare earth monopicnide family also includes YbAs, which was experimentally reported to be a topologically trivial semimetal under ambient pressure[6] and theoretically demonstrated to show band inversion under applied pressure of 6 GPa[7], turning it into a Z_2 topological insulator. In this study, we discussed the effect of pressure on topological phase of YbAs by implementing a more accurate hybrid functional with density functional theory (DFT). The invariants, calculated from the parity table of wave functions on high symmetry points, and Wannier Charge Centres (WCCs) along with existence of odd number of gapless topological surface states confirm the topological phase in YbAs.

2 Computational Details

Our calculations were based on the projector augmented wave (PAW) approach[8] as implemented in the VASP code[10]. The screened hybrid functional of HSE06[11] was used to calculate the exchange-correlation potential. The plane wave basis set had a kinetic energy cutoff of 380 eV and 7x7x7 k-mesh applied to sample the Brillouin zone (BZ). The maximally localised Wannier functions (MLWFs)[12] were used to construct the TB Hamiltonian and surface band structure. The Wannier charge centers (WCCs) were obtained using the Wannier Tools code[13].

3 Result & Discussions

At ambient pressure, the NaCl-type (space group $Fm\bar{3}m$) structure of YbAs have (0, 0, 0) and (1/2, 1/2, 1/2) position coordinates for As and Yb, respectively, as illustrated in Fig. 1(a). The optimized lattice parameter (5.722 Å), structural phase transition (SPT) and dynamical stability of NaCl-type structure of YbAs with applied hydrostatic pressure is discussed in our previous report[7]. The band structure of YbAs at normal pressure is shown in Fig. 1(c). K-path for band structure includes the Time Reversal Invariant Momenta (TRIM) points in the BZ (*i.e.*, X, Γ and L). A small overlap between the valance and conduction bands around the Fermi level (Fig. 1(b)), in the orbital projected density of states (PDOS), demonstrated that YbAs is semimetallic in nature which is fully agree with previous experimental study[6]. The band structure, Fig. 1(c), indicates that YbAs is a topologically trivial and the *p*-orbital of As dominate in valance band and the *d*-orbital of Yb dominate in

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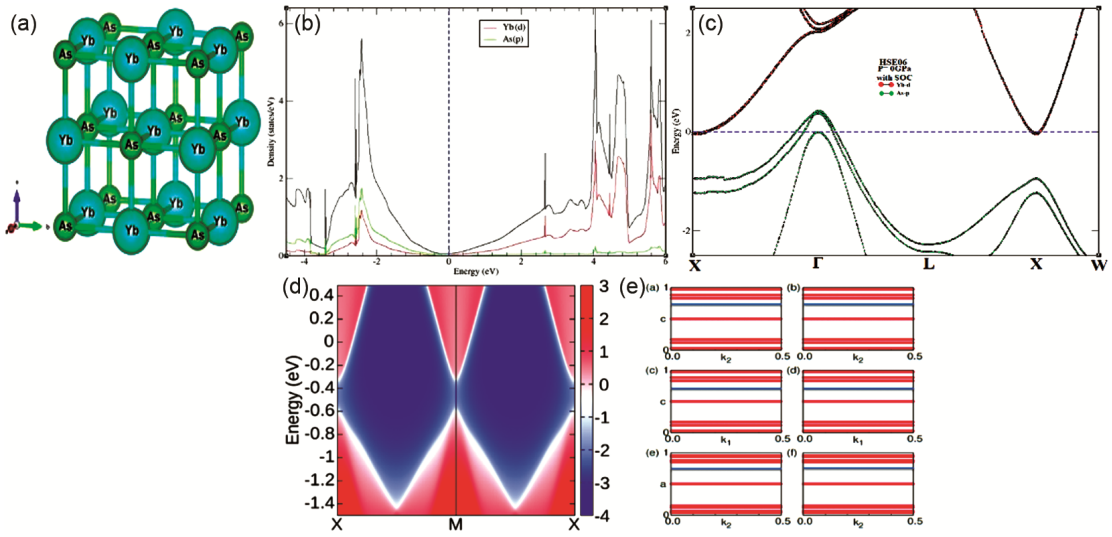

Fig.1 — (a) NaCl-type structure, (b) Orbital projected density of states (PDOS), (c) Orbital projected band structure, (d) Surface density of states (SDOS), (e) wannier change centers (WCCs), of YbAs at ambient pressure (P=0 GPa). The Fermi energy is set at 0 eV.

conduction band near the Fermi level. There is no evidence of a band inversion near Fermi level, at ambient pressure, as it was reported experimentally using angle-resolved photoemission spectroscopy (ARPES) measurement[6]. So, the true nature of YbAs at ambient pressure has been anticipated by our investigation which also confirmed by SDOS and WCCs in Fig. 1(d) & (e). We raised the external hydrostatic pressure inside the SPT limit to investigate the topological quantum phase transition in semimetal YbAs.

External pressure leads to change in lattice parameter, which influences the energy width between bands without changing charge neutrality of the YbAs. We examined the band inversion at each TRIM point to look for the sign of a topological quantum phase transition. Unlike to earlier findings[7], we observed that the band structure of YbAs does not change adiabatically from 0 to 19.5 GPa and retains its trivial state. As we increased the pressure from 19.5 to 20 GPa, we discovered a band inversion at the X point (shown by the bold arrow in Fig. 2(a)). With applied hydrostatic pressure, the elevation in SOC takes place which results this inversion at X point. The presence of the C_{4v} double group[3] at the X point in the rock salt structure of YbAs indicates that it contains both time and space inversion symmetries. To further confirm the quantum phase transition, we have examined the parity of the bands close to the Fermi level at the X TRIM point. The band parities at ambient pressure and 20 GPa are listed in Table 1. Applied hydrostatic pressure of 20 GPa switch the parities at X TRIM point near Fermi level which verifies the band inversion. It appears that YbAs is not a Dirac semimetal due to the opening of the band gap at the X point with inversion (inset of Fig. 2(a)). Table 1 shows that all three X point in BZ have opposite parities, implying that YbAs may be a topological insulator described on curved Fermi surface[3]. However, at 20 GPa, an inverted contribution of the *d*-orbital of Yb in valance band and *p*-orbital of As in conduction band can be observed at X point near the Fermi level (Fig. 2(a)). Additionally, we derived Z_2 topological invariants as described by Kane and Mele[14] to confirm the non-trivial topological phase of YbAs under applied hydrostatic pressure of 20 GPa. There are eight distinct TRIM points for three-dimensional systems that may be expressed as:

$$G_{i=(m_1 m_2 m_3)} = (m_1 a_1 + m_2 a_2 + m_3 a_3)/2 \quad \ldots (1)$$

where m_j = 0,1 and the reciprocal primitive lattice vectors are a_1, a_2, and a_3. Four Z_2 indices (ν_0; ν_1, ν_2, ν_3) can be examined with the help of change in the sign of parity to identify adiabatic change in the band structure. The following relationship between parity and Z_2 indices can be used to determine ν_0:

$$(-1)^{\nu_0} = \prod_{m_j=0,1} \delta m_1 m_2 m_3 \quad \ldots (2)$$

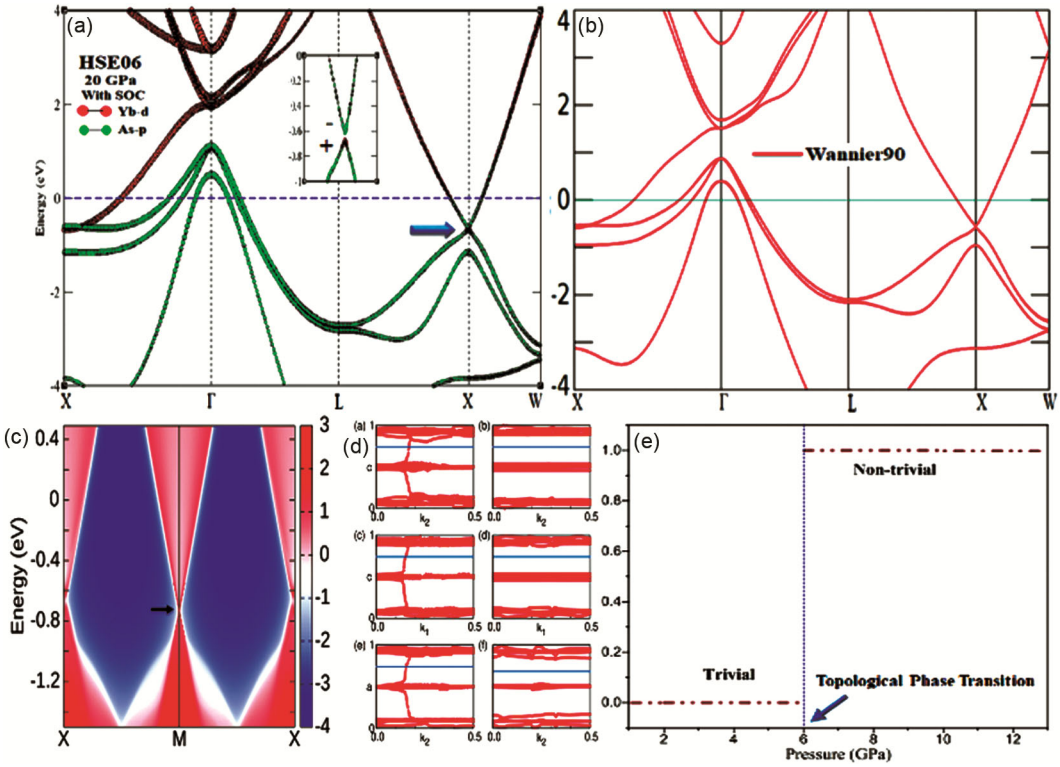

Fig.2 — (a)Orbital projected band structure,(b)wannierized band structure,(c) Surface density of states (SDOS),(d) wannier change centers (WCCs),(e) first Z_2 topological index,w.r.t. hydrostatic pressure of YbAs at P=20 GPa. The Fermi energy is set at 0 eV.

Table 1 — Parity table of YbAs at 0 GPa and 20 GPa.

TRIMs Pressure	4L	Γ	3X	$\prod \delta_m$	Z_2
0 GPa	-	+	+	+	0
20 GPa	-	+	-	-	1

where δ_i signifies the parities of all the filled bands at all TRIM points. YbAs is topologically trivial since there is no band inversion at ambient pressure and which can be verified with ν_0 value 0 calculated from at the X point when we apply 20 GPa pressure and it turns ν_0 into 1, indicating a topologically non-trivial phase. Fig. 2(e) shows the change in the first Z_2 topological index as a function of pressure. We computed the (001) surface band structure to further illustrate the topologically nontrivial nature of YbAs under hydrostatic pressure. YbAs exhibits bulk band inversion at three X TRIM points, showing three Dirac cones on the surface states associated with the inversions. These Dirac cones related to band in version are projected onto the surface Brillouin zone. These three X TRIM points are projected on M point in surface Brillion zone (SBZ). In Fig. 2(c), surface Dirac cone is shown along X-M-X k-path. To examine the topological phase and Z_2 topological invariants of YbAs, we calculate WCCs on six $k_i = 0, \pi$ (i = x, y, z)TRIM planes. The behaviour of WCCs for six in variant planes along given k-path is shown in Fig. 1(e) & 2(d).

Fig. 2(d) shows odd number of crossings of WCCs with horizontal reference line on $k_i = 0$ planes in half Brillion zone (BZ) which verifies the non-trivial topological phase with the invariant $Z_2 = 1$. Even number of crossings of WCCs with horizontal reference line in Fig. 1(e) with $k_i = 0, \pi$ planes and in Fig. 2(d) with $k_i = \pi$ planes show a trivial phase with the invariant $Z_2 = 0$. Four distinct 3D topological invariants (ν_0; $\nu_1\nu_2\nu_3$) = (1;000) have been identified with the help of the parity table (Table 1) and WCCs (Fig. 2(b) & Fig. 4(b)), which confirms the non-trivial phase of YbAs protected by TRS at a hydrostatic pressure of 20 GPa.

4 Conclusion

We have discovered the non-trivial topological phase of experimentally synthesized YbAs under applied hydrostatic pressure. Our First-principles calculations have shown that YbAs is topologically trivial at ambient pressure with SOC. The strength of SOC in system enhanced due to applied hydrostatic pressure resulting in a topological phase change from trivial to a non-trivial at 20 GPa. We have investigated the (001) surface states where the

characteristic crossing can be observed. We have found that YbAs hosts three Dirac cones along three X TRIM points which are projected to M point in surface Brillion zone. Band inversion has been confirmed by an exchange of orbital contribution in bands close to the Fermi level under pressure. The calculation of Z_2 indices or Z_2 topological invariants has established the topological phase transition. Product of parities and WCCs shows the change from zero to non-zero in first Z_2 topological invariant at 20 GPa pressure. This has shown that over the mentioned pressure value, a topologically non-trivial state of YbAs can be achieved.

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