Lorentz-violating type-II Dirac fermions in full-Heusler compounds XMg$_2$Ag ($X = Pr, Nd, Sm$)

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Abstract
Lorentz-violating type-II Dirac fermion, as a new type of quasiparticles beyond the high-energy physics, has received intense attention recently. However, excellent candidate materials which contain sufficiently more type-II Dirac points near the Fermi level are still in scarcity. Here, we report a family of existing full-Heusler compounds, namely XMg$_2$Ag ($X = Pr, Nd, Sm$), can serve as excellent Lorentz-violating type-II Dirac semimetals. We find they show several symmetry-protected nodal loops and triply degenerate nodal points (TDNPs) when spin–orbit coupling (SOC) is not considered. These fermions show clear nontrivial surface states. When SOC is included, the TDNPs transform into type-II Dirac points, characterized by Fermi arc surface states. The type-II DPs are protected by the $C_4$ symmetry in the $\Gamma$–$X$ path. Comparing with other type-II Dirac semimetals, XMg$_2$Ag compounds have additional advantages including: (i) they contain as much as three pairs of type-II Dirac points; (ii) all the Dirac points locate very close to the Fermi level. These advantages make XMg$_2$Ag compounds are suitable for studying the novel properties of type-II Dirac fermions in future experiments.

1. Introduction

In recent years, Dirac and Weyl fermions have brought intense research interests in both the high-energy physics and the condensed-matter physics [1–23]. Dirac fermion happens in system which preserves both the inversion symmetry ($P$) and the time-reversal ($T$) symmetry and is formed by the linear crossing between two doubly degenerate bands near Fermi level [1–7]. If the $T$ symmetry or the $P$ symmetry is broken, the Dirac point can split into one pair of Weyl points with opposite chiralities, thereby transforms into Weyl semimetals [8–21]. The Weyl points are formed by the crossing between two non-degenerate bands. In the three-dimensional (3D) momentum space, a Weyl fermion shows the positive or negative charge magnetic monopole. The low-energy excited Dirac (Weyl) fermions follow the Dirac (Weyl) equations and can generate many interesting physical phenomena, such as chiral anomaly [24] and quantum magnetoresistance [25].

Unlike in the high-energy physics, the Lorentz invariance is not required in the condensed matter physics [26]. This brings the possibilities of realizing new types of fermionic states in realistic materials. Indeed, Lorentz-violating fermions, namely type-II fermions, have been firstly proposed in Weyl semimetals [8–13]. Such proposal is not limited to constructed models, but also has been identified in several realistic materials [13–21]. Especially, type-II Weyl fermions have been already confirmed by experiments in MoTe$_2$ [17] and WTe$_2$ [21] compounds. Most importantly, type-II Weyl fermion is proposed to show unique properties that the type-I counterpart does not have, such as the modified anomalous Hall conductivity [27], unconventional quantum oscillations and novel Klein tunneling [28–30]. Comparing with type-II Weyl fermions, the studies for type-II Dirac fermions are much less. One major reason is that, excellent
candidate materials for type-II Dirac semimetals are still limited. To the best of our knowledge, type-II Dirac semimetals have been only proposed in few materials including RbMgBi [5], VAl₃ [6], PtSe₂ materials [4], and superconducting YPd₂Sn classe [7]. Among them, only PtSe₂ materials have been confirmed in experiments [31]. However, the type-II Dirac points in PtSe₂ materials locate quite far away from the Fermi level (at $-1.86$ eV to $-2.54$ eV), which are almost unavailable for future applications in electronics. Therefore, exploring excellent type-II Dirac semimetals with Dirac points sufficiently close to the Fermi level is in urgent need.

In this work, we report a new class of type-II Dirac semimetals in existing full-Heusler compounds XMg₂Ag ($X = Pr, Nd, Sm$). We find these compounds show quite similar band structures. Without considering spin–orbit coupling (SOC), they show three pairs of type-II triple degeneracy nodal points (TDNPs) and two nodal loops near the Fermi level. The TDNP and nodal loop fermions exhibit clear surface states. Remarkably, the TDNPs transform into type-II Dirac points when SOC is included. They contain three pairs of type-II Dirac points along three equivalent high-symmetry $k$-paths $Γ−X$ in Brillouin zone (BZ). The presence of these Dirac points is protected by the $C_{4v}$ symmetry. All the Dirac points locate very close to the Fermi level, thus XMg₂Ag compounds can be well described as Lorentz-violating type-II Dirac semimetals.

2. Computational methods

The electronic band structures of XMg₂Ag ($X = Pr, Nd, Sm$) compounds are calculated under the framework of density functional theory (DFT) by using the Vienna ab initio Simulation Package (VASP) [32, 33]. The exchange-correlation potential is chosen as the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) functional [34]. The cut-off energy is set as 500 eV. The whole BZ is sampled with the $Γ$-centered $k$ mesh of $15 \times 15 \times 15$. During the lattice optimization, the force and energy convergence criteria are set as 0.01 eV Å⁻¹ and $10^{-3}$ eV, respectively. The surface states are obtained by using the WannierTools package [35, 36] and the iterative Green’s function method [37], as implemented in the WannierTools package [38].

3. Results and discussions

The full-Heusler XMg₂Ag ($X = Pr, Nd, Sm$) compounds have been synthesized since 1988 and were found to be stable in ambience condition [39–41]. They share the cubic crystal structure with the space group Fm-3m (No. 225), as shown in the figure 1(a). In the structure, $X$ ($X = Pr, Nd, or Sm$) and Ag atoms constitute the NaCl-type local structure and two Mg atoms occupy the next-nearest-neighbor sites. This structure is known as the $L2₁$-type Heusler structure. In the structure, Ag, Mg and $X$ atoms occupy the 4$c$ Wyckoff sites $(0, 0, 0), (0.25, 0.25, 0.25), (0.5, 0.5, 0.5)$, respectively. As shown in table 1, the optimized lattice constants are very close to the experimental values [39]. In the following, we use the optimized lattice constants to investigate the electronic band structures of XMg₂Ag compounds. To be noted, the conclusions of this work will not change if the experimental lattice constants are applied.

In figures 2(a) and (b), we show electronic band structures of XMg₂Ag compounds without and with considering SOC, respectively. We find these compounds all show metallic band structures with several bands crossing the Fermi level. As shown by the total and projected density of states in figure 1(c), the electronic states near the Fermi level are found to be mostly contributed by the $f$ orbitals of $X$ ($X = Pr, Nd, Sm$) atoms in XMg₂Ag compounds. In their band structures without SOC [see figure 2(a)], there show several linear band crossing points in the high-symmetry $k$-paths $Γ−X, X−U$ and $K−Γ$. We will demonstrate later that, these band crossings form nodal loops and TDNPs. When SOC is taken into account, some of the band crossings are gapped and leave several pairs of symmetry-protected type-II Dirac points in the $k$-path $Γ−X$ [see figure 2(b)]. Considering the $f$ orbitals of the rare-earth elements (Pr, Nd and Sm), we have also checked our results by employing the GGA + $U$ calculations [42, 43]. We find the band structures are nearly unchanged at different $U$ values (see supplementary information https://stacks.iop.org/NJP/22/073061/mmedia), thus we here employ the GGA calculations. Noticing that the band structures for these XMg₂Ag compounds are quite similar, in the following we use PrMg₂Ag compound as an example to investigate the topological band structure of XMg₂Ag compounds.

We first discuss the band structure without SOC. The enlarged electronic band structure along the $k$-paths $Γ−X−U$ and $K−Γ$ for PrMg₂Ag is shown in figure 3(a). In the band structure, we can observe three band crossings near the Fermi level: $P_1$ in the $Γ−X$ path at $−0.235$ eV; $P_2$ in the $X−U$ path at $0.045$ eV; and $P_3$ in the $K−Γ$ path at $0.18$ eV. By carefully examining the band degeneracy near the crossing point $P_1$, we find it is in fact a TDNP, as formed by the crossing between non-degenerate band and a doubly-degenerate
Figure 1. (a) Crystal structure and (b) the bulk and the (001) surface Brillouin zone of full-Heusler compounds XMg2Ag (X = Pr, Nd, Sm). (c) The total and projected density of states (PDOS) of XMg2Ag compounds without considering SOC. 

Table 1. Calculated and experimental lattice constants of XMg2Ag (X = Pr, Nd, Sm) compounds. The locations of type-II Dirac points along the high-symmetry k-path Γ–X in the BZ (kx), and their relative energies (ED) with respect to the Fermi energy.

| Compounds       | Calculate: a = b = c Å | Experimental: a = b = c kx (π/a) | ED (eV) |
|-----------------|------------------------|----------------------------------|---------|
| PrMg2Ag         | 5.103                  | 5.13 Å [39]                      | 0.3850  |
| NdMg2Ag         | 5.086                  | 5.13 Å [39]                      | 0.3874  |
| SmMg2Ag         | 5.048                  | 5.13 Å [39]                      | 0.3851  |

Based on symmetry analysis, it is found that the two bands for the TDNP show two inequivalent irreducible representations Γ3 and Γ5 of the C4v double group. Considering the crystal symmetry, there totally possess three pairs of such TDNPs along the Γ–X paths, as shown in figure 3(b). These TDNPs situate at (±0.192, 0.00, 0.00), (0.00, ±0.192, 0.00), (0.00, 0.00 ± 0.192) in the BZ, locating at about 0.23 eV below the Fermi level. Just like Weyl/Dirac points, TDNPs can also be termed into type-I, type-II and critical type [44], based on the slopes of the crossing bands near TDNPs. Most TDNPs proposed previously are type-I, such as TiB2 family [45], ZrTe class [46], and ScSnPt family [47]. In addition, Jin et al proposed the nearly critical type TDNPs in Li2NaN [44]. However, type-II TDNPs have been rarely proposed in realistic materials. Very interestingly, we find the TDNPs in PrMg2Ag belong to type-II, as clearly shown in figure 3(a).

Next, we discuss the other two crossing points P2 and P3 in the X–U and K–Γ paths. Unlike the triple band degeneracy in P1, crossing points P2 and P3 both have the double band degeneracy. Symmetry analysis shows that the two bands for P2 have inequivalent irreducible representations Γ2 and Γ1 of the C2v symmetry, and the two bands for the P3 have irreducible representations Γ3 and Γ4 of the C2v symmetry. Besides, considering XMg2Ag compounds preserve have both the T and P symmetries, crossing points P2 and P3 cannot be discrete nodal points, based on the arguments by Weng et al [48]. This has been verified by our DFT calculations. We find that the crossing point P2 resides on a nodal loop in the U–Γ–X plane, centering the Γ point in the BZ. Crossing point P3 belongs another nodal loop in the kz = 0 plane, centering the X point. In the following, we denote the former nodal loop as NL1, and the latter one as NL2. The profiles of NL1 and NL2 are shown in figure 3(c). We can observe that, NL1 shows a petal shape and NL2 shows an elliptical shape. The locations of the nodal loops in the BZ are schematically shown in figure 3(d). It is well known that, nodal loops are usually characterized by drumhead-like surface states. In figures 3(e) and (f), we show the (001) surface spectrum along the high-symmetry k-paths W–Γ–W′ and Γ–X–U respectively. For the two cases, NL1 can be projected in the k-path W–Γ–W′, and NL2 is projected
Figure 2. Electronic band structures of full-Heusler compounds XMg$_2$Ag ($X =$ Pr, Nd, Sm) without (a) and with (b) SOC, respectively. The $E_D$ in (b) denotes the locations of energy for the type-II Dirac points. In (a) and (b), the energy at the Fermi level is set as zero.

Figure 3. (a) Electronic band structure along the high-symmetry $k$-paths $\Gamma-X-U$, and $K-\Gamma$ without SOC for PrMg$_2$Ag. The crossing points along the $\Gamma-X$, $X-U$ and $K-\Gamma$ paths are denoted as $P_1$, $P_2$, $P_3$, respectively. The energy at the Fermi level is set as zero. The irreducible representations for the crossing bands are provided. (b) The positions of the three pairs of type-II TDNPs (the green points) in the bulk Brillouin zone. (c) The profiles of the two nodal loops (denoted as NL1 and NL2) in PrMg$_2$Ag. (d) The locations of the two nodal loops in the bulk Brillouin zone. (e) and (f) show the (001) surface band structure of PrMg$_2$Ag along different $k$-paths. (e) and (f) are provided to show the surface states for NL1 and NL2, respectively. In (e) and (f), the red points show the positions of nodal points in the bulk bands and the arrows point the drumhead surface states.

in the $k$-path $\Gamma-X-U$. We indeed observe the drumhead-like surface states for the two nodal loops, as pointed by the arrows in figures 3(e) and (f).

In the following, we discuss the SOC effect on the electronic band structure. Figure 4(a) shows the electronic band structure along the $k$-paths $\Gamma-X-U$ and $K-\Gamma$ with SOC included for PrMg$_2$Ag. We find the band structure experience significant changes under SOC. First, the bands near crossing point $P_1$ in the
Figure 4. (a) Enlarged band structure along the high-symmetry \( k \)-paths \( \Gamma -X \) and \( K-\Gamma \) under SOC. (b) Shows the enlarged band structure near \( P_1 \). In the \( \Gamma -X \) path, the band crossing point is denoted as \( P_4 \). The energy at the Fermi level is set as zero. The irreducible representations for the crossing bands are provided. (c) The locations of three pairs of type-II Dirac points (the black points) in the bulk Brillouin zone. (d) The three-D plotting of the bands near the type-II Dirac point. (e) The (001) surface band structure of PrMg\(_2\)Ag. In (e), the black points show the positions of Dirac points in the bulk bands, and the arrows point the Fermi Arc surface states.

\( \Gamma -X \) path are fully split. Second, the crossing points \( P_2 \) and \( P_3 \) (which form nodal loops NL1 and NL2) are both gapped by SOC. The gap sizes at \( P_2 \) and \( P_3 \) are about 120 meV and 30 meV, respectively. Such SOC gaps are lower or comparable with typical nodal loop materials including Cu\(_3\)NPd (60–100 meV) [49, 50], CaAgBi (80–140 meV) [51], and BaSn\(_2\) materials (60–160 meV) [52]. Since \( P_2 \) and \( P_3 \) are fully gapped, in the following we will focus our attention on the band structure near \( P_1 \).

As highlighted by the box in figure 4(a), the triple band degeneracy at \( P_1 \) is fully split by SOC. Such band splitting seems to produce two new crossing points. We show the enlarged band structure of this region in figure 4(b). We can find in figure 4(b) that, the two bands in higher energy level indeed form a band crossing point (denoted as \( P_4 \)), while those in lower energy level in fact show a tiny band gap (about 1 meV). In PrMg\(_2\)Ag compound, it preserves both \( T \) and \( P \) symmetries, thus each band has a double degeneracy under SOC. Therefore, the crossing point \( P_4 \) in the \( \Gamma -X \) path is in fact a Dirac point (DP).

Symmetry analysis indicates that, the two bands for the DP show two inequivalent irreducible representations \( \Gamma_6 \) and \( \Gamma_7 \) of the \( C_{4v} \) double group, which protects the DP from opening gap. Considering the crystal symmetry in PrMg\(_2\)Ag, there totally contain three pairs of such symmetry-protected DPs along the \( \Gamma -X \) path, which situate at \((\pm 0.196, 0.00, 0.00), (0.00, \pm 0.196, 0.00), (0.00, 0.00 \pm 0.196)\) in BZ, as shown in figure 4(c). The position and energy \( (E_D) \) of DPs in these XMg\(_2\)Ag compounds have been summarized in table 1.

After a careful examination on the slopes of crossing bands at DPs [see figures 2(b) and 4(b)], we find the DPs in XMg\(_2\)Ag compounds all belong to type-II, with the electron-like and hole-like bands coexist at certain energy levels. Figure 4(d) shows the 3D plotting of band dispersion around the DP. We can clearly observe Dirac cone is tilted over, which is typical for type-II Dirac semimetals. These results suggest XMg\(_2\)Ag compounds can be well described as Lorentz-violating type-II Dirac semimetals, which are drastically different with conventional Dirac semimetals such as Na\(_3\)Bi [1] and Cd\(_3\)As\(_2\) [2]. In figure 5(e), we show the surface states of PrMg\(_2\)Ag projected onto the (001) surface. We can observe Fermi arcs connected to a pair of DPs. To date, type-II Dirac semimetals are only proposed in few realistic materials including VAl\(_3\), PtSe\(_2\) and YPd\(_2\)Sn class [5–7]. The XMg\(_2\)Ag compounds proposed here can greatly enrich the candidates for type-II Dirac semimetals.

Generally, Dirac semimetal state can be considered as a critical state for different phase transitions. We show this point in PrMg\(_2\)Ag by slightly shifting the crystal symmetry, where different topological phase transitions can be realized. As demonstrated above, the DPs in PrMg\(_2\)Ag are protected by the \( C_{4v} \) symmetry in the \( \Gamma -X \) path. Here, we break the \( C_{4v} \) symmetry by applying a small (1%) stress along the \( k_y \) direction, as shown in figure 5(a). The resulting band structure along the \( \Gamma -X \) path is shown in figure 5(d). We can find the DP is gapped with the \( C_{4v} \) symmetry broken, namely, PrMg\(_2\)Ag has transform from type-II Dirac semimetal state to an insulator state. Usually, one DP can split into a pair of Weyl points with the \( T \) or \( P \) symmetry broken. In PrMg\(_2\)Ag, we break the \( P \) symmetry by shifting four Mg atoms with 0.05 Å along the \( k_y \) direction, as shown in figure 5(c). The corresponding band structure is shown in figure 5(f). Indeed, each type-II DP has split into one pair of
Figure 5. (a) Breaking the $C_{4v}$ symmetry by applying a 1% stress along the $k_y$ direction on the PrMg$_2$Ag lattice, making the lattice constants $a \neq b = c$. (b) The native crystal structure of PrMg$_2$Ag. (c) Breaking the $P$ symmetry by shifting four Mg atoms with 0.05 Å along the $k_y$ direction in PrMg$_2$Ag. (d)–(f) are the corresponding band structures for (a), (b), and (c), respectively. In (f), the solid and hollow circles represent the ‘positive’ and ‘negative’ Weyl nodes.

type-II Weyl points (WP$_1$ and WP$_2$) with opposite chiralities. In this case, PrMg$_2$Ag has transformed from type-II Dirac semimetal to type-II Weyl semimetal state. These examples provide good platform to investigate different topological phase transitions in realistic materials.

Before closing, we have one crucial remark. The type-II Dirac Fermions in Heusler compounds XMg$_2$Ag are quite suitable for experimental detection, because they have following advantages. First, they are very easy to be synthesized and are stable. Second, they contain three pairs of type-II DPs, and the signal from Dirac Fermions is expected to be very pronounced, while most Dirac semimetals proposed previously only contain on pair of type-II DPs [4–6]. Third, the DPs happen very close to the Fermi level (at about 150 meV–190 meV below the Fermi level). Finally, the highly-ordered Heusler compounds quite favor the experimental detections on topological materials. For example, a large number of Heusler compounds have been convinced as topological insulators and topological superconductors from various experimental approaches such as angle-resolved photoemission spectroscopy (ARPES), transports, and nuclear magnetic resonance (NMR) [53–59]. We believe the type-II Dirac Fermions in Heusler compounds XMg$_2$Ag are also promising to be successfully detected by these experimental approaches.

Before closing, we have one crucial remark. Quite recently, we come aware to a superior work [60], which has pointed out the nontrivial band topology of XMg$_2$Ag compounds. It sweeps through 39 519 materials available in crystal database and identifies 8056 topological materials, listed in a topological database. Furthermore, the database has classified these materials into five categories. For XMg$_2$Ag compounds, as three among the 8056 materials, the database qualitatively classifies them into the high-symmetry-point semimetal (HSPSM) and high-symmetry-line semimetal (HSLSM) categories, but the definite topological signature is unknown. In current work, we systematically investigated the topological signature of XMg$_2$Ag materials under different conditions including without and with SOC and potential topological phase transitions under train. The TDNP and nodal line states without SOC, the type-II Dirac states under SOC and the topological phase transitions under strain and atomic engineering are reported here for the first time.

4. Summary

In summary, the topological band structures of XMg$_2$Ag (X = Pr, Nd, Sm) Heusler compounds have been systematically studied by using DFT calculations. Without considering SOC, we find XMg$_2$Ag compounds show three pairs of type-II TDNPs in $\Gamma$–X path and two nodal loops at different planes near the Fermi level. The TDNPs are protected the $C_{4v}$ symmetry without SOC, and are characterized with Fermi arc surface states. The nodal loops are protected by the $P$ and $I$ symmetries and are characterized with drumhead surface states. When SOC is taken into account, the nodal loops open small gaps, and the TDNPs have transformed into type-II DPs. These results suggest XMg$_2$Ag compounds can be well described as type-II Dirac semimetals. The type-II DPs are protected by the $C_{4v}$ symmetry under SOC and show Fermi arc surface states. We also show one type-II DP can further split into a pair of type-II Weyl points if the $P$
symmetry is broken. Since the XMg$_2$Ag Heusler compounds are easy to synthesis and stable, and contain as much as three pairs of DPs near the Fermi level, the novel properties associated with type-II Dirac Fermions are quite promising to be detected by experimental approaches such as ARPES, transport measurements and NMR.

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