Dirac nodal lines and induced spin Hall effect in metallic rutile oxides

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We have found Dirac nodal lines (DNLs) in the band structures of metallic rutile oxides IrO2, OsO2, and RuO2 and revealed a large spin Hall conductivity contributed by these nodal lines, which explains a strong spin Hall effect (SHE) of IrO2 discovered recently. Two types of DNLs exist. The first type forms DNL networks that extend in the whole Brillouin zone and appears only in the absence of spin-orbit coupling (SOC), which induces surface states on the boundary. Because of SOC-induced band anti-crossing, a large intrinsic SHE can be realized in these compounds. The second type appears at the Brillouin zone edges and is stable against SOC because of the protection of nonsymmorphic symmetry. Besides reporting new DNL materials, our work reveals the general relationship between DNLs and the SHE, indicating a way to apply Dirac nodal materials for spintronics.

I. INTRODUCTION

Topological semimetals are an emerging topological phase that has attracted great attention of the condensed-matter community in recent years. Their conduction and valence bands cross each other through robust nodal points or nodal lines in the momentum space. Distinct from normal semimetals or metals, resultant Fermi surfaces can be characterized by nontrivial topological numbers, giving rise to exotic quantum phenomena such as Fermi arcs on the surface, chiral anomaly in the bulk, anomalous Hall effect (AHE), and spin Hall effect (SHE). In this article, we have theoretically investigated the topology of the band structure of metallic rutile oxide IrO2 and similar oxides RuO2 and OsO2. We observe two types of DNLs in their band structures. The first type extends the whole BZ and forms a square-like DNL network in the absence of SOC, resulting in

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surface states. Joint points of the network are six- and eight-band-crossing points at the center and boundary of the BZ, respectively. These DNLs become gapped and lead to a strong SHE when SOC exists. The second type is stable against SOC and appears at the edges of the tetragonal BZ, which is protected by nonsymmorphic symmetries.

II. METHODS

To investigate the band structure and the intrinsic SHE, we have performed ab initio calculations based on the density-functional theory (DFT) with the localized atomic orbital basis and the full potential as implemented in the full-potential local-orbital (FPLO) code [58]. The exchange-correlation functionals were considered at the generalized gradient approximation (GGA) level [59]. We adopted the experimentally measured lattice structures for RO\(_2\) (R = Ir, Os, and Ru) compounds. By projecting the Bloch states into a highly symmetric atomic orbital like Wannier functions (O-p orbitals), we constructed tight-binding Hamiltonians and computed the intrinsic spin Hall conductivity (SHC) by the linear-response Kubo formula approach in the clean limit [53 60],

\[
\sigma_{ij}^k = \frac{e}{\hbar} \int_{BZ} \frac{d\tilde{k}}{(2\pi)^3} \sum_n f_{nk} \Omega_{n,ij}^k(\tilde{k}),
\]

\[
\Omega_{n,ij}^k(\tilde{k}) = -2i\hbar \sum_{n' \neq n} <n\tilde{k}|J^k_n|n'\tilde{k}^*><n'\tilde{k}^*|v_j|n\tilde{k}> (E_{n\tilde{k}} - E_{n'\tilde{k}})^2
\]

(1)

where \(f_{nk}\) is the Fermi–Dirac distribution for the \(n\)-th band. The spin current operator is \(J^k_n = \frac{1}{2} \{ v_i, s_p \}\), with the spin operator \(s\), the velocity operator \(v_i = \frac{1}{\hbar} \frac{\partial H}{\partial \tilde{k}_i}\), and \(i, j, k = x, y, z\). \(n\tilde{k}^*\) is the eigenvector for the Hamiltonian \(H\) at the eigenvalue \(E_{n\tilde{k}}\). \(\Omega_{n,ij}^k(\tilde{k})\) is referred as the spin Berry curvature as analogy to the ordinary Berry curvature. A 500 × 500 × 500 \(k\)-grid in the BZ was used for the integral of the SHC. The SHC \(\sigma_{ij}\) refers to the spin current \((j_{i,j}^{s,k})\), which flows along the \(i\)-th direction with the spin polarization along \(k\), generated by an electric field \((E_j)\) along the \(j\)-th direction, i.e., \(j_{i,j}^{s,k} = \sigma_{ij}^k E_j\).

III. RESULTS AND DISCUSSIONS

A. Nonsymmorphic symmetry

Three compounds RO\(_2\) (R = Ir, Os, and Ru) share the rutile-type lattice structure with space group P4\(_2/mnm\) (No. 136), as shown in Fig. 1. A primitive unit cell contains two \(R\) atoms that sit at the corner and center of the body-centered tetragonal lattice, respectively. One \(R\) atom is surrounded by six O atoms that form a distorted octahedron. For space group No. 136, we have the following generator operations,

\[
E, m_z, P, n_{x} \equiv \{m_x|\vec{r}\}, n_{yz} \equiv \{c_{4z}|\vec{r}\},
\]

where \(m_{x,z}\) are mirror reflections, \(c_{4z}\) is the four-fold rotation, \(P\) is the inversion symmetry, \(n_{x}\) and \(n_{yz}\) represent nonsymmorphic symmetries, and \(\vec{r} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\) is the translation of one-half of a body diagonal. Additionally; the time-reversal symmetry \(T\) also appears for RO\(_2\) systems.

It is known that electronic bands are doubly degenerate (considering spin and SOC) at every \(k\)-point of the BZ owing to the coexistence of \(P\) and \(T\). Furthermore, a generic nonsymmorphic symmetry leads to new band crossings and thus higher degeneracies at the BZ boundary. Therefore, the coexistence of \(P\), \(T\), and

![Fig. 1](image-url)
nonsymmorphic symmetries guarantees four-fold or even larger degeneracies at some k-points of the BZ boundary.

As discussed in the following, IrO$_2$ exhibits a four-fold degeneracy at the BZ edge lines, $X(Y) - M$ and $M - A$ (also see Fig. 1d). Consequently, one requires 4n electrons for filling these bands to obtain a band insulator. However, a primitive unit cell contains two IrO$_2$ formula units and in total 42 valence electrons, failing to satisfy the precondition of a band insulator in this nonsymmorphic space group [25, 61]. Therefore, IrO$_2$ is constrained by the lattice symmetry to be a band metal in the weak interaction case. Recently, it has been reported that IrO$_2$ cannot become a Mott insulator because of a large bandwidth [62, 63], while several seemingly similar iridates (e.g., Sr$_2$IrO$_4$) are known as 5$d$ Mott insulators with the $J_{\text{eff}} = 1/2$ state [63, 65].

B. Dirac Nodal lines without SOC

We first investigate the band structures without including SOC. As shown in Fig. 1c, six-band and eight-band crossing points (including spin) appear at the $\Gamma - Z$ and $M - A$ axes, respectively, which are noted as a hexatruple point (HP) and an octuple point (OP), respectively. There is a DNL connecting neighboring HP and OP in the BZ, forming a network in the $k$-space, as indicated by Figs. 1b and 3a. Two layers of networks are present above and below the $k_z = 0$ plane respectively, and can be transformed to each other by $P$ or $T$. DNLs exist inside the (110) and (110) mirror planes and originate from crossing of $d_{x^2-y^2}$ and $d_{xy}$ bands. Here, $d_{x^2-y^2}$ and $d_{xy}$ bands are all doubly degenerate owing to $P$ and $T$ and exhibit opposite eigenvalues $-1$ and $+1$, respectively, for each mirror reflection. The mirror symmetry protects the four-band-crossing in the absence of SOC.

The topology of a DNL is characterized by the nontrivial Berry phase (or winding number) along a closed path that includes the DNL. We choose a loop, along which the system is fully gapped as indicated in Fig. 1b [58, 61]. The Berry phase for all “occupied” bands is found to be a quantized value, $\pi$. This nonzero Berry phase further leads to surface states. When projecting to the (001) surface, the nodal band structure exhibits a local energy gap between $M$ and $X$ in the surface BZ. Two layers of DNL networks overlap in the (001) surface projection. Thus, one can observe two sets of surface states (spinless) connecting OPs between two adjacent $M$ points inside the gap in Fig. 2a.

When SOC is included and the $SU(2)$ symmetry is broken, these DNLs including HPs and OPs are gapped (see Fig. 1d), since there is no additional symmetry protection. On the surface, original spinless surface states split into two Rashba-like spin channels (see Fig. 2b). Because of the lack of robust symmetry protection (e.g., $P$ is commonly breaking on the surface), these surface states may appear or disappear according to the surface boundary condition.

C. Dirac nodal lines with SOC

The $k_x = \pi$ and $k_y = \pi$ planes are actually Dirac nodal planes in the absence of SOC. The presence of SOC gaps these planes and only leaves DNLs along some high-symmetry lines, $X-M$ and $M-A$. By taking the DNL along $X-M$ as an example, we can understand the four-fold degeneracy by considering time reversal symmetry $T$, point group symmetries, $m_z$, $P$, and nonsymmorphic symmetry $n_z$. Since $[m_z, H] = 0$ in the $k_z = 0$ plane, we can choose the eigenstates of Hamiltonian $H$ with definite mirror parity for $\vec{k}$ along $X-M$,

$$H(\vec{k})|\phi_\alpha(\vec{k})\rangle = E_\pm(\vec{k})|\phi_\pm(\vec{k})\rangle$$

$$m_z|\phi_\pm(\vec{k})\rangle = \pm i|\phi_\pm(\vec{k})\rangle$$

where $i$ is from the spin. First, we know $[TP, m_z] = 0$. Therefore, we have

$$m_z(TP|\phi_\alpha(\vec{k})\rangle) = TP(m_z|\phi_\alpha(\vec{k})\rangle)$$

$$= TP(i\alpha|\phi_\alpha(\vec{k})\rangle) = -i\alpha(TP|\phi_\alpha(\vec{k})\rangle)$$

where $\alpha = \pm 1$. Therefore, $TP|\phi_\alpha(\vec{k})\rangle$ is also an eigenstate at $\vec{k}$ ($TP\vec{k} = \vec{k}$) with the mirror parity $-i\alpha$, where $- -$ sign is from the complex conjugate in $T$. Next, we consider the commutation between $m_z$ and the glide mirror symmetry $n_x$, both of which act in real space ($x, y, z$) and the spin space simultaneously. In real space, we have

$$(x, y, z) \xrightarrow{n_z} (-x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2})$$

$$(m_z) \xrightarrow{n_z} (-x + \frac{1}{2}, y + \frac{1}{2}, -z - \frac{1}{2})$$

$$(x, y, z) \xrightarrow{m_z} (x, y, -z)$$

$$(n_z) \xrightarrow{m_z} (x, y, -z)$$

$$m_z n_z = T_{(0,0,-1)} n_z m_z$$

where $T_{(0,0,-1)} = e^{ik_z}$ is the translation operator when acting on the Bloch wavefunction. In the spin space, $m_z = i\sigma_z$ and $n_x = i\sigma_x$ and thus $m_z n_z = -n_z m_z$. By combining the real space and the spin space, we obtain

$$m_z n_z = e^{ik_z} (-1)n_z m_z$$

Therefore, $n_z|\phi_\alpha(\vec{k})\rangle$ is also an eigenstate at $\vec{k}$ ($n_z\vec{k} = \vec{k}$), but with a mirror parity $-i\alpha$. Further, the combination of $TPn_z$ leads to one more state $TPn_z|\phi_\alpha(\vec{k})\rangle$ with a mirror parity $+i\alpha$.

In total, we can have four eigenstates, $|\phi_\alpha(\vec{k})\rangle$, $TP|\phi_\alpha(\vec{k})\rangle$, $n_z|\phi_\alpha(\vec{k})\rangle$, and $TPn_z|\phi_\alpha(\vec{k})\rangle$ for
\(\vec{k} (\pi, k_y, 0)\) along \(X-M\). The mirror parities of \(m_z\) are \(+i\alpha\) for \(|\phi_{\alpha}(\vec{k})\rangle\) and \(TPn_x|\phi_{\alpha}(\vec{k})\rangle\), and \(-i\alpha\) for \(TP|\phi_{\alpha}(\vec{k})\rangle\) and \(n_x|\phi_{\alpha}(\vec{k})\rangle\). Next, we will prove that they are orthogonal to each other, i.e., two eigenstates with the same mirror parity are orthogonal, \(<\phi_{\alpha}(\vec{k})|TPn_x|\phi_{\alpha}(\vec{k})\rangle = 0\). This requires that \(TPn_x\) is anti-unitary. In real space, we have

\[
(x, y, z) \xrightarrow{Pn_z} (x - \frac{1}{2}, y - \frac{1}{2}, z - \frac{1}{2}) \quad \text{and} \quad \xrightarrow{TPn_z} (x - 1, y, z)
\]

In the spin space, \(P = 1\) and \(n_x = i\sigma_x\). Therefore, we have \((Pn_x)^2 = -e^{i\vec{k}z}\). Considering \(T^2 = -1\) for spinful fermions, we obtain \((TPn_x)^2 = e^{i\vec{k}z} = -1\) for \(\vec{k} = (\pi, k_y, 0)\). Since \(TPn_x\) is an anti-unitary operator that satisfies \(<\phi|\psi|TPn_x|\phi\rangle = <TPn_x|\psi|TPn_x|\phi\rangle\), we have

\[
<\phi_{\alpha}(\vec{k})|TPn_x|\phi_{\alpha}(\vec{k})\rangle = <(TPn_x)^2\phi_{\alpha}(\vec{k})|TPn_x|\phi_{\alpha}(\vec{k})\rangle = -<\phi_{\alpha}(\vec{k})|TPn_x|\phi_{\alpha}(\vec{k})\rangle = 0
\]

which means the states \(TP|\phi_{\alpha}(\vec{k})\rangle\) and \(n_x|\phi_{\alpha}(\vec{k})\rangle\) are orthogonal to each other.

Therefore, we prove that there are four degenerate orthogonal eigenstates along the \(X-M\) line. We point out that the nonsymmorphic symmetry is crucial to protect the four-fold degeneracy, while only \(P, T\), and \(m_z\) cannot stabilize DNLs. Likewise, we can also understand the four-fold degeneracy along the \(M-A\) line considering \(m_z\), \(P, T\), and another nonsymmorphic symmetry \(n_{4z}\).

These DNLs protected by nonsymmorphic symmetries are similar to those DNLs observed at the BZ edges in ZrSiS and HfSiS (e.g., [45, 66]). We find that the Berry phase along a loop (indicated in Fig. 1b) including such a DNL is zero. Therefore, we do not expect apparent topological surface states related to these DNLs. It is still interesting to point out that the density of states scales linearly to the energy for DNLs. Then one can expect different correlation effects in DNL semimetals from a nodal point semimetal and a normal metal [23, 67].

For IrO\(_2\), such DNLs appear at the Fermi energy, while they stay far below the Fermi energy in ZrSiS-type compounds. These DNLs may be responsible for the high conductivity and large magnetoresistance [68, 69].

### D. Dirac nodal lines and spin Hall effect

The first type of DNLs, DNL networks without SOC, indicate the existence of a strong SHE in RO\(_2\). It is known that band anti-crossing induced by SOC can lead to a large intrinsic SHE. To maximize the SHE, one needs to increase the number of band anti-crossing points, i.e., nodal points in the absence of SOC. Therefore, a DNL, an assembly of continual nodal points in the BZ, can induce a strong SHE. The DNL networks that constitute many DNLs will further enhance the SHE. Because such type of DNLs without SOC are usually protected by the mirror symmetry, it will be insightful to look for SHE materials in space groups that host many mirror or glide mirror planes. This argument seems consistent with the fact that current best SHE materials are usually Pt and W metals (e.g., [70, 71]) from the high-symmetry space groups.

Next, we compute the intrinsic SHE for RO\(_2\) compounds following Eq. [1] based on the band structure including SOC. The SHE \(\sigma^k_{ij}\) is a second-order tensor with 27 elements. The number of independent nonzero

\[
\begin{array}{c|ccc}
\text{IR} & \begin{bmatrix} \text{IrO}_2 & \text{OsO}_2 & \text{RuO}_2 \end{bmatrix} \\
\hline
\sigma^x_{yz} & 8 & 9 & 8y \\
\sigma^x_{zx} & -253 & -311 & -238 \\
\sigma^x_{yz} & -161 & -541 & -284 \\
\end{array}
\]

\(\text{FIG. 2. Surface band structure for IrO}_2\text{ projected to the (001) surface without (a) and with (b) SOC. The brightness of color represents the weight of surface states. (c) The projection of the bulk BZ to the surface BZ with DNLs.}\)
be seen from Table I. Here, the largest SHC of the three compounds, the SHC is very anisotropic, as can be seen from Table I. Here, the largest SHC of RO$_2$ is still smaller than that of Pt [$\sigma_{xy} \sim 2000(\hbar/e)(\Omega \cdot cm)^{-1}$]. However, RO$_2$ may exhibit a large spin Hall angle (the ratio of the SHC over the charge conductivity) owing to their high resistivity compared to a pure metal, as already found in IrO$_2$ [54].

Here, we also demonstrate the direct correspondence between DNLs and the SHC. Since the SHC is obtained by integrating the spin Berry curvature over the BZ, we show the distribution of $\Omega_{n,z}(\vec{k})$ in the (110) mirror plane that hosts DNLs. In the band structure along DNLs in Fig. 3, the SOC clearly gaps a DNL that connects a HP and an OP. Correspondingly, one can find two “hot lines” of the spin Berry curvature, which is the anti-crossing region of the DNLs. Thus, it is clear that the first-type DNLs contribute to a large SHC for IrO$_2$-type materials. In contrast, the second-type DNLs at the BZ edges (e.g., that along $M-A$ in Fig. 3c) show a slight contribution to the SHC.

IV. CONCLUSIONS

To summarize, we found two types of DNLs in metallic rutile oxides IrO$_2$, OsO$_2$, and RuO$_2$. First-type DNLs form networks that extend in the whole BZ and appear only in the absence of SOC, which induces surface states at the boundary. The second type of DNLs is stable against SOC because of the protection of nonsymmorphic symmetry. Because of the SOC-induced gap for first-type DNLs, a large intrinsic SHE can be realized in these compounds. This explains the strong SHE observed in IrO$_2$ in the previous experiment. Moreover, our calculation suggests that OsO$_2$ will behave even better than IrO$_2$ in SHE devices, as OsO$_2$ shows a larger intrinsic SHC. Our work implies that first-type DNLs (or nodal points that can be gapped by SOC) and the SHE may be commonly related to each other, indicating new guiding principles to search for DNLs in SHE materials or enhance the SHE by DNLs in the band structure. For example, it will be insightful to look for SHE materials in high-symmetry space groups with many mirror or glide mirror planes, which can induce the first type of DNLs.

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