

Discovering Topological Surface States of Dirac Points

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Dirac materials, unlike the Weyl materials, have not been found in experiments to support intrinsic topological surface states, as the surface arcs in existing systems are unstable against symmetry-preserving perturbations. Utilizing the proposed glide and time-reversal symmetries, we theoretically design and experimentally verify an acoustic crystal of two frequency-isolated three-dimensional Dirac points with Z_2 monopole charges and four gapless helicoid surface states.

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A three-dimensional (3D) Dirac point [1] disperses the same way as the solutions to the massless Dirac equation at the vicinity of the fourfold linear point degeneracy. Playing a central role in 3D band topology, Dirac points can, upon symmetry breaking, transition into Weyl points, line nodes or topological band gaps with gapless surface states. Although 3D Dirac points have been experimentally discovered in electron [2–7], magnon [8,9], and photonic [10] systems along with a variety of other theoretical proposals [11–23], none of the surface states are topological. Specifically, there have been no robust gapless surface bands associated with the bulk Dirac points [24–26].

The current lack of topological surface states for Dirac points can be understood through the anticrossing of two Weyl surface states. Illustrated in Fig. 1, the topological surface dispersion of a Weyl crystal is a doubly periodic helicoid sheet whose singularities locate at the projection of the bulk Weyl points. The chirality of the helicoid around each Weyl point equals the sign of its Chern number. Since a Dirac point is composed of two Weyl points of opposite Chern numbers, the Dirac surface state should be composed of two helicoids of opposite chiralities. Two opposite helicoid surfaces generally cross each other along a line of momenta and anticross (hybridize with each other), resulting in gapped surface bands which are topologically trivial. The only exception was theoretically proposed in Ref. [27], in which the glide symmetries combined with the time-reversal ($\mathcal{T}$) can stabilize a degenerate line and protect the crossing of the helicoids. As illustrated in Fig. 1, one glide can protect double helicoids and two glides can protect quad-helicoid surface states.

In this work, we present an acoustic band structure with two ideal Z_2 Dirac points protected by glide reflections. The acoustic crystal is 3D printed and the measured surface dispersions exhibit quad-helicoid surface sheets.

Ideal acoustic Dirac points.—The cubic cell of the acoustic crystal, in Fig. 2(a), consists of thick rods and thin sticks, belonging to space group $Ia\bar{3}$ (No. 206) of the body-centered-cubic (BCC) lattice. The four thick rods of radius $0.15a$ point at the directions of the BCC lattice vectors, where a is the lattice constant of the cubic cell. These disconnected rods form the blue phase I (of liquid crystal) photonic crystal in Refs. [28,29]. We add the thin sticks to connect all rods and mechanically support the whole structure. The sticks are too thin, $0.025a$ in radius to change the Dirac acoustic bands, as compared in the Supplemental Material [30]. The background material is air and the interfaces are treated as sound hard-wall boundaries in numerical simulations.

There are two Dirac points located at the $\pm P$ points of the BCC Brillouin zone [BZ, Fig. 2(b)], where four bands (from the fifth to the eighth in ascending energy order) meet, as shown in Fig. 2(c). The density of states (DOS) [31] vanishes at the Dirac frequency and grows quadratically away from it, as expected for linear dispersion relations.

The local Hamiltonian of this Dirac point is $H(\mathbf{k}) \sim \begin{pmatrix} k_\sigma & 0 \\ 0 & -k_\sigma \end{pmatrix}$, determined by the $\mathbf{k} \cdot \mathbf{p}$ analysis detailed in the Supplemental Material [30]. This fourfold degeneracy is joined, due to the antiunitary parity-time symmetry ($\mathcal{PT}$), by two conjugated 2D representations of the little group. The little group of No. 206 at P also has a fourfold representation which is the generalized Dirac point discussed in Refs. [28,29]. The Dirac point has identical group velocities while the generalized one does not.

Each Dirac point is stabilized by the products of $\mathcal{T}$ and the three noncommuting glides ($G_x = \{M_x|(a/2)\hat{x} + (a/2)\hat{y}\}$, $G_y = \{M_y|(a/2)\hat{x}\}$, $G_z = \{M_z|(a/2)\hat{y}\}$), denoted as $G_i\mathcal{T}$ ($i = x, y, z$). M_i are the mirror operations and the

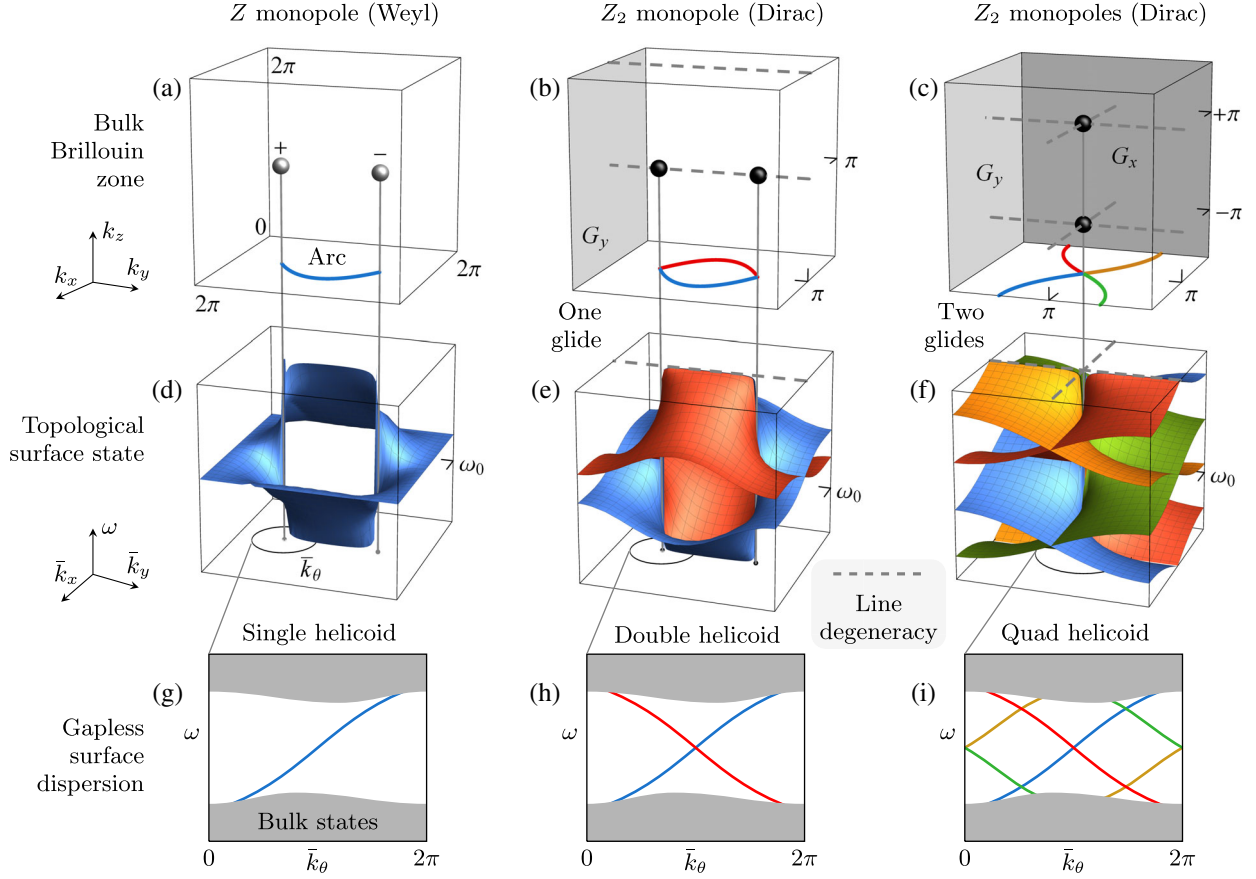


FIG. 1. Bulk monopoles and helicoid surfaces. (a), (b), (c) are the 3D BZ containing two Z or Z_2 monopoles. (a), (b) can be the BZs of cubic lattices, while (c) is the BZ of the BCC lattice in our acoustic design. The arcs, at the bottom plane, are the isofrequency contours of the helicoid surface states at frequency ω_0 labeled in (d), (e), (f). The glide planes are fill in gray and the G_iT protected line degeneracies are shown in dashed gray lines. (g), (h), (i) illustrate the gapless surface dispersions, around the projected monopoles, along a circular path of $\bar{k}_\theta$ in the surface BZ. The Z monopoles can be Weyl points, nodal lines, or surfaces. The Z_2 monopoles can be Dirac points, Z_2 nodal lines, or Weyl dipoles.

inversion $\mathcal{P} = G_x G_y G_z$. Each G_iT symmetry enforces a line degeneracy at the zone boundary, represented by the dashed lines in all figures consistently. The three degeneracy lines intersect at the P point, shown in Figs. 2(b) and 2(e). We note that the P points have neither T nor G_i symmetries by themselves.

Z_2 monopoles.—The Dirac point is the symmetry-protected Z_2 monopole in the 3D momentum space [32–34]. However, the Z_2 symmetries in these systems ($\mathcal{PT}$ for example) cannot protect any line degeneracies on the surface, disallowing the gapless connectivity between two helicoids of opposite chiralities. In contrast, the Z_2 invariant of our acoustic Dirac point is protected by G_iT [27], leading to the nontrivial band topology not only in the bulk, but also on the surface.

In Fig. 2(d), we calculate the non-Abelian Berry phase [35] of the lower two bands (5th and 6th) on a sphere enclosing the Dirac point. The gapless spectra indicate the nontrivial monopole charge of $Z_2 = 1$. Since this Z_2 charge can be protected by either one of the three G_iT [27], we can

break the other two or one G_iT to get the Z_2 nodal ring [36–40] and Weyl dipoles [27,32,41]. These symmetry-breaking cases are illustrated in Figs. 2(e), 2(f) and 2(g) and are discussed in detail in the Supplemental Material [30].

Quad-helicoid and Jacobi elliptic function.—We project the two Dirac points onto the (001) surface, corresponding to the case in Figs. 1(c), 1(f) and 1(i). The plane group of this surface is $p2gg$, on which the two degenerate lines due to G_xT and G_yT are presented. These two line degeneracies, outlining the whole boundaries of the surface BZ, protect all the crossings among the four helicoid surface sheets. The isofrequency contours, in Fig. 1(c), are four branches originating from the projected Dirac points. The four branches are connected across the zone boundary forming two noncontractible loops.

If we parametrize the 2D surface BZ as a complex plane ($z \propto k_x + ik_y$) [27], the helicoid surface bands can be expressed as (are topologically equivalent to) the double-periodic elliptic functions [42,43]. The four helicoids in Fig. 1(f) are plotted using the Jacobi elliptic functions

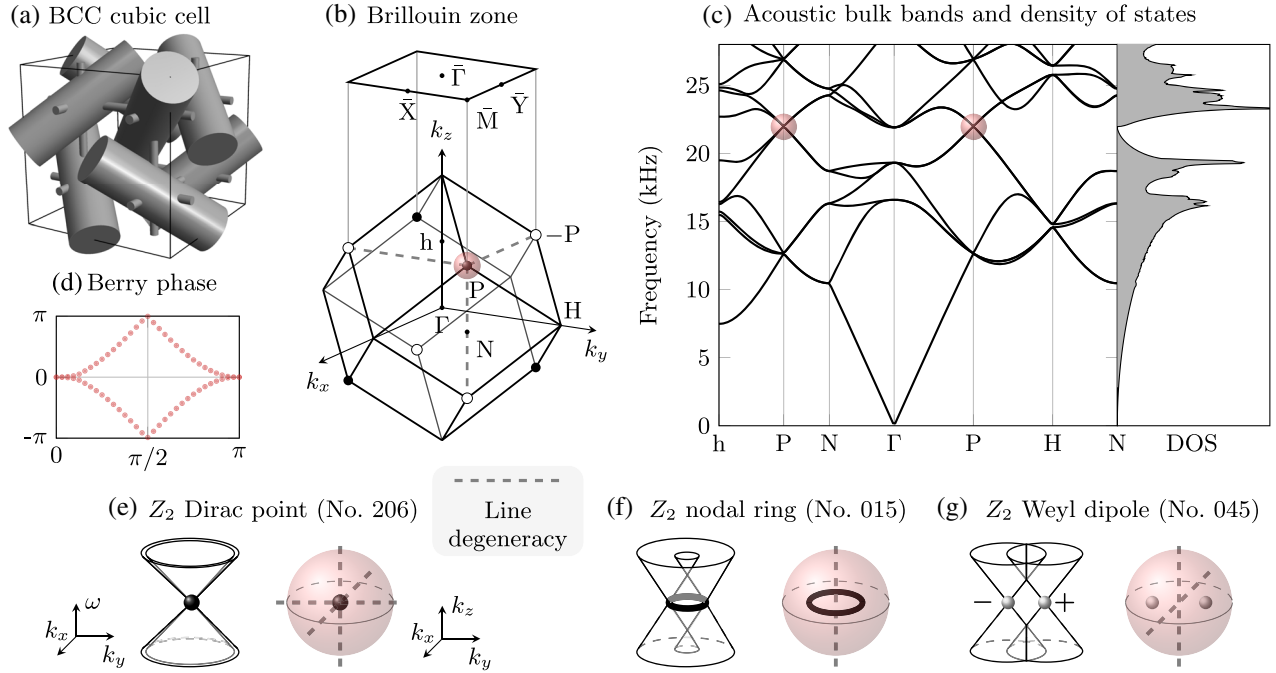


FIG. 2. Ideal acoustic Dirac points with Z_2 charges. (a) One cubic cell of the acoustic crystal of BCC lattice. (b) BCC BZ and the [001] surface BZ. The two $\pm P$ points project to the same point $\bar{M}$ in the surface BZ. (c) Acoustic bulk band structure with the Dirac points crossing between the 5th and 6th bands and the 7th and 8th bands at the P point. The DOS vanished at the frequency of ideal Dirac points. (d) Calculated non-Abelian Berry phases on the surface of the red sphere enclosing the Dirac point. Over the polar angle, the nontrivial winding of Berry phases implies the topological invariant of $Z_2 = 1$. (e), (f), (g) Three types of four-band nodal structures that carry Z_2 monopole charges. The dashed gray lines are the line degeneracies due to $G_i T$, and the red spherical surfaces enclose the Z_2 monopoles.

$cn(z, \frac{1}{2})$. The Jacobi function has two zeros and two poles in one period, each locating at the center of each quadrant. These four singularities represent two Weyl dipoles, and all project to the same point in the surface BZ. So, we construct the quad-helicoid surfaces by stacking the four quadrants of the Jacobi function and align the central singularities. The mapping of one quadrant is $\omega(k_x, k_y) \sim \text{Im}(\log\{cn[z_i(k_x, k_y), \frac{1}{2}]\})$, where $z_1(k_x, k_y) = [K(\frac{1}{2})/\pi][k_x - k_y/2 + i(k_x + k_y/2)]$ and K is the complete elliptic integrals of the first kind. The rest of the three quadrants are obtained by the translations of $z_2(k_x, k_y) = z_1(k_x + 2\pi, k_y)$, $z_3(k_x, k_y) = z_1(k_x, k_y + 2\pi)$, and $z_4(k_x, k_y) = z_1(k_x + 2\pi, k_y + 2\pi)$.

Experiments.—A photograph of the Dirac acoustic crystal is shown in Fig. 3(a), 3D printed by the stereo lithography method using photocurable resin. The lattice constant is $a = 20$ mm and the fabrication error is ± 0.1 mm. The total size of the sample is $413.0 \times 413.0 \times 222.8$ mm containing $20 \times 20 \times 11$ cubic cells.

The surface states are measured through the Fourier-transformed field scan (FTFS). Similar approaches have been used to study other topological acoustic crystals [44–48]. A pressure-field microphone (diameter of 3.5 mm, B&K-4138-A-015) is used as the scanning probe (receiver). The microphone is embedded in an aluminum alloy plate

which works as a hard wall boundary on the top surface of the sample, as shown in Fig. 3(a). The acoustic source is a broadband earphone, having frequency response up to 40 kHz and a diameter of 5.5 mm, fixed at the corner of the sample close to the plate. The amplitude and phase of the pressure field are collected by the data acquisition module B&K-3160-A-042. A broadband signal is generated from the module and split into two channels, one to drive the earphone and the other as a time reference for the receiver. The frequency spectrum is averaged 100 times for each point scan and is normalized by the signal from the source.

The field scan is performed by moving the sample stage in three directions. During the collection of each data point, the sample is pressed towards the top plate to ensure the absence of air gaps. The scanning step is 5 mm and the scanning range is 400 mm in both x and y directions. Through 2D Fourier transforms, we obtain the spectral weight of the surface states in the momentum range of $(-2, 2) 2\pi/a$. Similar to the processing technique used in Ref. [49], we patch the data of spatial scans to double the momentum resolution in the reciprocal space. In the x direction, we stitch two scanning fields of equivalent source positions. In the y direction, we rotate the data due to the C_2 symmetry on the surface.

The FTFS results are shown in three plots in Figs. 3(d), 3(f), and 3(h). The corresponding numerical results of the

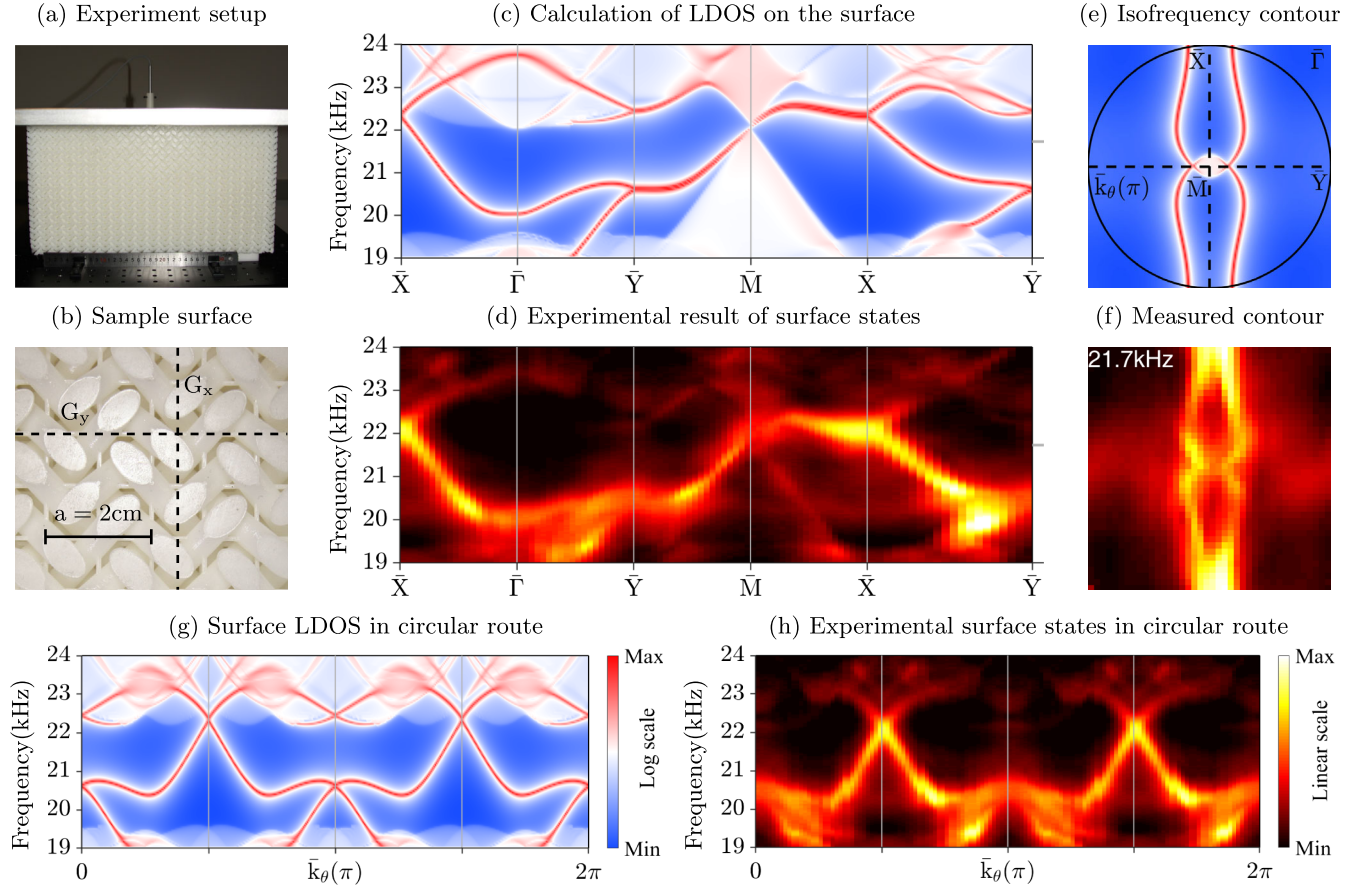


FIG. 3. Experiment observation of the quad-helicoid surface states by FTFS. (a) Photograph of the 3D-printed sample on the measurement setup. (b) Photograph of the sample surface. (c), (d) Numerical and experimental results of the surface states on the high-symmetry momentum lines. (e), (f) Numerical and experimental isofrequency contour of the quad-helicoid surfaces showing four branches at 21.7 kHz. (g), (h) Numerical and experimental results of the surface states in a circular route around the projected bulk Dirac points.

local DOS (LDOS)[50] at the measurement interface are shown in Figs. 3(c), 3(e), and 3(g), respectively. The detailed algorithm of the surface LDOS will be presented in a separate paper. The agreement between experiments and numerics are visually obviously for the gapless surface dispersions.

Discussion.—We experimentally observed the first example of topological surface states associated with the 3D Dirac points, while there is no topological edge states associated with the 2D Dirac points. The line degeneracy due to glide and $\mathcal{T}$ symmetry are the keys for stabilizing the gapless connection of helicoid sheets of opposite chiralities. Similarly, the other nonsymmorphic symmetry (screw rotation) and $\mathcal{T}$ could also protect such line degeneracies when a domain wall is constructed to preserve the screw axis on the surface. It will also be interesting to explore the material realization of the double-helicoid surface states shown in Fig. 1(e), as well as helicoid surface states of Dirac semimetals [27].

This work establishes an ideal 3D Dirac material for consequent studies. For example, symmetry breakings of Dirac points can generate a variety of topological phenomena,

such as the charged (Z or Z_2) nodal lines, nodal surfaces [51,52], Weyl dipoles, as well as a gapped bulk state supporting gapless surface [28] or chiral hinge modes [53,54].

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Note added in the proof.—We noticed a similar work [55].

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- [1] N. P. Armitage, E. J. Mele, and A. Vishwanath, Weyl and Dirac semimetals in three-dimensional solids, *Rev. Mod. Phys.* **90**, 015001 (2018).
- [2] Z. K. Liu, B. Zhou, Y. Zhang, Z. J. Wang, H. M. Weng, D. Prabhakaran, S.-K. Mo, Z. X. Shen, Z. Fang, X. Dai *et al.*,

- Discovery of a three-dimensional topological Dirac semimetal, Na_3Bi , *Science* **343**, 864 (2014).
- [3] M. Neupane, S. Y. Xu, R. Sankar, N. Alidoust, G. Bian, C. Liu, I. Belopolski, T. R. Chang, H. T. Jeng, H. Lin, A. Bansil, F. Chou, and M. Z. Hasan, Observation of a three-dimensional topological Dirac semimetal phase in high-mobility Cd_3As_2 , *Nat. Commun.* **5**, 3786 (2014).
 - [4] Z. K. Liu, J. Jiang, B. Zhou, Z. J. Wang, Y. Zhang, H. M. Weng, D. Prabhakaran, S. K. Mo, H. Peng, P. Dudin, T. Kim, M. Hoesch, Z. Fang, X. Dai, Z. X. Shen, D. L. Feng, Z. Hussain, and Y. L. Chen, A stable three-dimensional topological Dirac semimetal Cd_3As_2 , *Nat. Mater.* **13**, 677 (2014).
 - [5] S. Borisenko, Q. Gibson, D. Evtushinsky, B. B. Zabolotnyy, and R. J. Cava, Experimental Realization of a Three-Dimensional Dirac Semimetal, *Phys. Rev. Lett.* **113**, 027603 (2014).
 - [6] S. Y. Xu, C. Liu, S. K. Kushwaha, R. Sankar, J. W. Krizan, I. Belopolski, M. Neupane, G. Bian, N. Alidoust, T. R. Chang, H. T. Jeng, C. Y. Huang, W. F. Tsai, H. Lin, P. P. Shibayev, F. C. Chou, R. J. Cava, and M. Z. Hasan, Observation of fermi arc surface states in a topological metal, *Science* **347**, 294 (2015).
 - [7] H. Yi *et al.*, Evidence of topological surface state in three-dimensional Dirac semimetal Cd_3As_2 , *Sci. Rep.* **4**, 6106 (2015).
 - [8] W. Yao, C. Li, L. Wang, S. Xue, Y. Dan, K. Iida, K. Kamazawa, K. Li, C. Fang, and Y. Li, Topological spin excitations in a three-dimensional antiferromagnet, *Nat. Phys.* **14**, 1 (2018).
 - [9] S. Bao, J. Wang, W. Wang, Z. Cai, S. Li, Z. Ma, D. Wang, K. Ran, Z.-Y. Dong, D. L. Abernathy, S.-L. Yu, X. Wan, J.-X. Li, and J. Wen, Discovery of coexisting Dirac and triply degenerate magnons in a three-dimensional antiferromagnet, *Nat. Commun.* **9**, 2591 (2018).
 - [10] Q. Guo, O. You, B. Yang, J. B. Sellman, E. Blythe, H. Liu, Y. Xiang, J. Li, D. Fan, J. Chen, C. T. Chan, and S. Zhang, Observation of Three-Dimensional Photonic Dirac Points and Spin-Polarized Surface Arcs, *Phys. Rev. Lett.* **122**, 203903 (2019).
 - [11] S. M. Young, S. Zaheer, J. C. Y. Teo, C. L. Kane, E. J. Mele, and A. M. Rappe, Dirac Semimetal in Three Dimensions, *Phys. Rev. Lett.* **108**, 140405 (2012).
 - [12] Z. Wang, Y. Sun, X. Chen, C. Franchini, G. Xu, H. Weng, X. Dai, and Z. Fang, Dirac semimetal and topological phase transitions in $A_3\text{Bi}$ ($A = \text{Na}, \text{K}, \text{Rb}$), *Phys. Rev. B* **85**, 195320 (2012).
 - [13] Z. Wang, H. Weng, Q. Wu, X. Dai, and Z. Fang, Three-dimensional Dirac semimetal and quantum transport in Cd_3As_2 , *Phys. Rev. B* **88**, 125427 (2013).
 - [14] J. A. Steinberg, S. M. Young, S. Zaheer, C. L. Kane, E. J. Mele, and A. M. Rappe, Bulk Dirac Points in Distorted Spinels, *Phys. Rev. Lett.* **112**, 036403 (2014).
 - [15] H. X. Wang, L. Xu, H. Chen, and J.-H. Jiang, Three-dimensional photonic Dirac points stabilized by point group symmetry, *Phys. Rev. B* **93**, 235155 (2016).
 - [16] P. Tang, Q. Zhou, G. Xu, and S.-C. Zhang, Dirac fermions in an antiferromagnetic semimetal, *Nat. Phys.* **12**, 1100 (2016).
 - [17] G. Li, B. Yan, Z. Wang, and K. Held, Topological Dirac semimetal phase in Pd and Pt oxides, *Phys. Rev. B* **95**, 1 (2017).
 - [18] A. Slobozhanyuk, S. H. Mousavi, X. Ni, D. Smirnova, Y. S. Kivshar, and A. B. Khanikaev, Three-dimensional all-dielectric photonic topological insulator, *Nat. Photonics* **11**, 130 (2017).
 - [19] Q. Guo, B. Yang, L. Xia, W. Gao, H. Liu, J. Chen, Y. Xiang, and S. Zhang, Three Dimensional Photonic Dirac Points in Metamaterials, *Phys. Rev. Lett.* **119**, 213901 (2017).
 - [20] H.-X. Wang, Y. Chen, Z. H. Hang, H.-Y. Kee, and J.-H. Jiang, Type-II Dirac photons, *npj Quantum Mater.* **2**, 54 (2017).
 - [21] C. Le, X. Wu, S. Qin, Y. Li, R. Thomale, F. Zhang, and J. Hu, Dirac semimetal in $\beta\text{-CuI}$ without surface fermi arcs, *Proc. Natl. Acad. Sci. U.S.A.* **115**, 8311 (2018).
 - [22] P. Zhang *et al.*, Multiple topological states in iron-based superconductors, *Nat. Phys.* **15**, 41 (2019).
 - [23] Y. Yang, Z. Gao, H. Xue, L. Zhang, M. He, Z. Yang, R. Singh, Y. Chong, B. Zhang, and H. Chen, Realization of a three-dimensional photonic topological insulator, *Nature (London)* **565**, 622 (2019).
 - [24] M. Kargarian, M. Randeria, and Y.-M. Lu, Are the surface fermi arcs in Dirac semimetals topologically protected, *Proc. Natl. Acad. Sci. U.S.A.* **113**, 8648 (2016).
 - [25] M. Kargarian, Y.-M. Lu, and M. Randeria, Deformation and stability of surface states in Dirac semimetals, *Phys. Rev. B* **97**, 165129 (2018).
 - [26] Y. Wu, N. H. Jo, L.-L. Wang, C. A. Schmidt, K. M. Neilson, B. Schunk, P. Swatek, A. Eaton, S. L. Bud'ko, P. C. Canfield, and A. Kaminski, Fragility of fermi arcs in Dirac semimetals, *Phys. Rev. B* **99**, 161113 (2019).
 - [27] C. Fang, L. Lu, J. Liu, and L. Fu, Topological semimetals with helicoid surface states, *Nat. Phys.* **12**, 936 (2016).
 - [28] L. Lu, C. Fang, L. Fu, S. G. Johnson, J. D. Joannopoulos, and M. Soljačić, Symmetry-protected topological photonic crystal in three dimensions, *Nat. Phys.* **12**, 337 (2016).
 - [29] L. Lu, C. Fang, T. H. Hsieh, L. Fu, S. G. Johnson, J. D. Joannopoulos, and M. Soljačić, Generalized three-dimensional Dirac points and z_2 gapless surface states in a topological photonic crystal, in *CLEO:2015* (Optical Society of America, 2015), p. FTh3D.7.
 - [30] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevLett.124.104301>, for detailed $\mathbf{k} \cdot \mathbf{p}$ analysis, symmetry-breaking realizations and more numerical and experimental data.
 - [31] B. Liu, J. D. Joannopoulos, S. G. Johnson, and L. Lu, Generalized Gilat-Raubenheimer method for density-of-states calculation in photonic crystals, *J. Opt.* **20**, 044005 (2018).
 - [32] T. Morimoto and A. Furusaki, Weyl and Dirac semimetals with Z_2 topological charge, *Phys. Rev. B* **89**, 235127 (2014).
 - [33] B.-J. Yang and N. Nagaosa, Classification of stable three-dimensional Dirac semimetals with nontrivial topology, *Nat. Commun.* **5**, 4898 (2014).
 - [34] B.-J. Yang, T. Morimoto, and A. Furusaki, Topological charges of three-dimensional Dirac semimetals with rotation symmetry, *Phys. Rev. B* **92**, 165120 (2015).
 - [35] R. Yu, X. L. Qi, A. Bernevig, Z. Fang, and X. Dai, Equivalent expression of Z_2 topological invariant for band insulators using the non-Abelian berry connection, *Phys. Rev. B* **84**, 075119 (2011).

- [36] C. Fang, Y. Chen, H.-Y. Kee, and L. Fu, Topological nodal line semimetals with and without spin-orbital coupling, *Phys. Rev. B* **92**, 081201 (2015).
- [37] K. Li, C. Li, J. Hu, Y. Li, and C. Fang, Dirac and Nodal Line Magnons in Three-Dimensional Antiferromagnets, *Phys. Rev. Lett.* **119**, 247202 (2017).
- [38] T. Bzdušek and M. Sigrist, Robust doubly charged nodal lines and nodal surfaces in centrosymmetric systems, *Phys. Rev. B* **96**, 155105 (2017).
- [39] Z. Song, T. Zhang, and C. Fang, Diagnosis for Nonmagnetic Topological Semimetals in the Absence of Spin-Orbital Coupling, *Phys. Rev. X* **8**, 031069 (2018).
- [40] J. Ahn, D. Kim, Y. Kim, and B.-J. Yang, Band Topology and Linking Structure of Nodal Line Semimetals with Z_2 Monopole Charges, *Phys. Rev. Lett.* **121**, 106403 (2018).
- [41] E. V. Gorbar, V. A. Miransky, I. A. Shovkovy, and P. O. Sukhachov, Surface Fermi arcs in Z_2 Weyl semimetals A_3Bi ($A = Na, K, Rb$), *Phys. Rev. B* **91**, 235138 (2015).
- [42] T. Zhang, Z. Song, A. Alexandradinata, H. Weng, C. Fang, L. Lu, and Z. Fang, Double-Weyl Phonons in Transition-Metal Monosilicides, *Phys. Rev. Lett.* **120**, 016401 (2018).
- [43] B. Yang, Q. Guo, B. Tremain, R. Liu, L. E. Barr, Q. Yan, W. Gao, H. Liu, Y. Xiang, J. Chen *et al.*, Ideal Weyl points and helicoid surface states in artificial photonic crystal structures, *Science* **359**, 1013 (2018).
- [44] F. Li, X. Huang, J. Lu, J. Ma, and Z. Liu, Weyl points and fermi arcs in a chiral phononic crystal, *Nat. Phys.* **14**, 30 (2018).
- [45] H. Ge, X. Ni, Y. Tian, S. K. Gupta, M.-H. Lu, X. Lin, W.-D. Huang, C. T. Chan, and Y.-F. Chen, Experimental Observation of Acoustic Weyl Points and Topological Surface States, *Phys. Rev. Applied* **10** (2018).
- [46] Y. Yang, H. x. Sun, J. p. Xia, H. Xue, Z. Gao, Y. Ge, D. Jia, S. q. Yuan, Y. Chong, and B. Zhang, Topological triply degenerate point with double fermi arcs, *Nat. Phys.* **15**, 645 (2019).
- [47] V. Peri, M. Serra-Garcia, R. Ilan, and S. D. Huber, Axial-field-induced chiral channels in an acoustic Weyl system, *Nat. Phys.* **15**, 357 (2019).
- [48] B. Xie, H. Liu, H. Cheng, Z. Liu, S. Chen, and J. Tian, Experimental Realization of Type-II Weyl Points and Fermi Arcs in Phononic Crystal, *Phys. Rev. Lett.* **122**, 104302 (2019).
- [49] Q. Yan, R. Liu, Z. Yan, B. Liu, H. Chen, Z. Wang, and L. Lu, Experimental discovery of nodal chains, *Nat. Phys.* **14**, 461 (2018).
- [50] M. P. Lopez Sancho, J. M. Lopez Sancho, J. M. L. Sancho, and J. Rubio, Highly convergent schemes for the calculation of bulk and surface green functions, *J. Phys. F* **15**, 851 (1985).
- [51] M. Xiao, L. Ye, C. Qiu, H. He, Z. Liu, and S. Fan, Experimental demonstration of acoustic semimetal with topologically charged nodal surface, *Sci. Adv.* **6**, eaav2360 (2020).
- [52] Y. Yang, J. Xia, H. Sun, Y. Ge, D. Jia, S. Yuan, S. Yang, Y. Chong, and B. Zhang, Observation of a topological nodal surface and its surface-state arcs in an artificial acoustic crystal, *Nat. Commun.* **10**, 5185 (2019).
- [53] C. Yue, Y. Xu, Z. Song, H. Weng, Y.-M. Lu, C. Fang, and X. Dai, Symmetry-enforced chiral hinge states and surface quantum anomalous hall effect in the magnetic axion insulator $Bi_{2-x}Sm_xSe_3$, *Nat. Phys.* **15**, 577 (2019).
- [54] H. Kim, K. Shiozaki, and S. Murakami, Glide-symmetric magnetic topological crystalline insulators with inversion symmetry, *Phys. Rev. B* **100**, 165202 (2019).
- [55] X. Cai, L. Ye, C. Qiu, M. Xiao, R. Yu, M. Ke, Z. Liu, Symmetry-enforced three-dimensional Dirac phononic crystals, *arXiv:2001.06191*.

Discovering topological surface states of Dirac points: Supplementary material

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I. UNIT CELL DESIGN

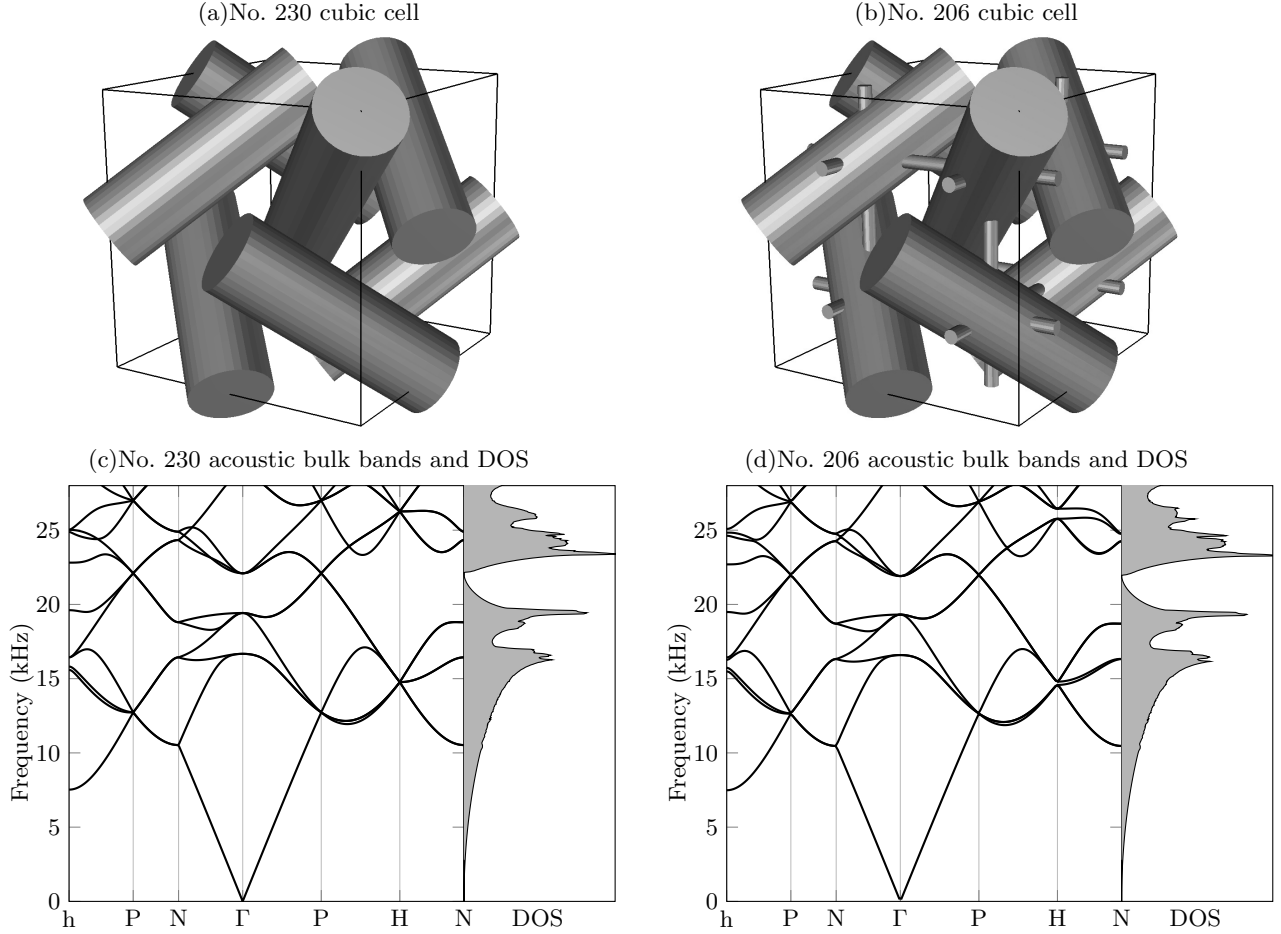


FIG. S1: Design of ideal acoustic Dirac point without and with the thin sticks. (a), (c) BPI acoustic crystal of space group No. 230. (b), (d) Thin-stick joined BPI acoustic crystal of space group No. 206.

For sample stability, we add the 12 thin sticks of diameter $0.05a$ (1 mm in experiment) to connect all the BPI rods. Fig. S1(a), (b) are the unit-cell structures without and with thin sticks, they belong to space group No. 230 and No. 206 respectively. The thin sticks preserve the three glides that protect the ideal Dirac points. The corresponding acoustic bulk bands are plotted in Fig. S1(c), (d), which are almost identical for the frequency range of the Dirac points.

II. $\mathbf{k} \cdot \mathbf{p}$ MODEL

The local dispersion and topology at P point can be described by the effective Hamiltonian of $\mathbf{k} \cdot \mathbf{p}$ model, written as $H(\mathbf{k}) = A\mathbf{k} \cdot \mathbf{p}$, considering the first non-zero order of $\mathbf{k}$. Here, we show the detailed derivation of the effective Hamiltonian of our ideal acoustic Dirac point in space group $Ia\bar{3}d$ (No. 230) and $Ia\bar{3}$ (No. 206).

Considering the space group $Ia\bar{3}d$ (No. 230), we choose four independent symmetry operations (generators) of the little group at momentum point P . They are two-fold rotation symmetry $C_{2z} = \{C_2|(0, \frac{1}{2}, 0)\}$ along $[001]$ direction, two-fold rotation symmetry $C_{2y} = \{C_2|(\frac{1}{2}, 0, 0)\}$ along $[010]$ direction, three-fold rotation symmetry C_3 along $[111]$ direction and glide reflection symmetry $G = \{M|(-\frac{3}{4}, -\frac{3}{4}, \frac{1}{4})\}$ in $[1\bar{1}0]$ plane. Here G is different from the G_i ($i = x, y, z$) glides in $[100]$, $[010]$, $[001]$ planes. P point has no G_i ($i = x, y, z$) symmetries, but has $G_i\mathcal{T}$ that can be obtained by $G_i\mathcal{T} = C_{2i} \cdot \mathcal{PT}$ ($i = x, y, z$). $\mathcal{PT}$ is the parity-time symmetry preserves in the whole BZ.

P point has $\mathcal{PT}$ but has neither $\mathcal{P}$ nor $\mathcal{T}$. $\mathcal{PT}$ is an anti-unitary operator which can be written as $\mathcal{PT} = U \cdot \mathcal{K}$, where U is a unitary matrix and $\mathcal{K}$ is the complex conjugate. The little group of P point has two conjugated 2D representations, forming a 4D representation under $\mathcal{PT}$. We obtain the irreducible representation (Irrep) matrices of the selected generators from Bilbao crystal server, noted as Bilbao Rep. in Table II. After unitary transformations, we have the representation matrices in real basis (Real Rep.) and in Dirac basis (Dirac Rep.).

Operators	Bilbao Rep.	Real Rep.	Dirac Rep.
C_{2z}	$\begin{pmatrix} i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & -i \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & -i \end{pmatrix}$
C_{2y}	$\begin{pmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
C_3	$\frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\frac{3}{4}\pi} & e^{i\frac{7}{4}\pi} & 0 & 0 \\ e^{i\frac{5}{4}\pi} & e^{i\frac{5}{4}\pi} & 0 & 0 \\ 0 & 0 & e^{i\frac{3}{4}\pi} & e^{i\frac{7}{4}\pi} \\ 0 & 0 & e^{i\frac{5}{4}\pi} & e^{i\frac{5}{4}\pi} \end{pmatrix}$	$\frac{1}{2} \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \end{pmatrix}$	$\frac{-1}{2} \begin{pmatrix} 1-i & -1-i & 0 & 0 \\ 1-i & 1+i & 0 & 0 \\ 0 & 0 & 1-i & -1-i \\ 0 & 0 & 1-i & 1+i \end{pmatrix}$
G	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -i & 0 \end{pmatrix}$	$\frac{-1}{2} \begin{pmatrix} 0 & 1+i & 0 & 1+i \\ 1+i & 0 & -1-i & 0 \\ 0 & -1-i & 0 & 1+i \\ 1+i & 0 & 1+i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -1 & 0 \\ 0 & -i & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$
$\mathcal{PT}$	$\Gamma_{22}\mathcal{K}$	$\mathcal{K}$ (complex conjugate)	$\Gamma_{22}\mathcal{K}$
$H(\mathbf{k})$	$(\sigma_x + w\sigma_y) \otimes (k_z\sigma_z + k_x\sigma_y - k_y\sigma_x)$	$(-k_x\Gamma_{10} - k_y\Gamma_{33} + k_z\Gamma_{31}) + w(-k_x\Gamma_{30} + k_y\Gamma_{13} - k_z\Gamma_{11})$	$\sqrt{1+w^2}\sigma_z \otimes \mathbf{k} \cdot \boldsymbol{\sigma}$
mass	$m\Gamma_{30} + m'(\Gamma_{20} - w\Gamma_{10})$	$m\Gamma_{20} + m'(\Gamma_{32} - w\Gamma_{12})$	$m\Gamma_{10} + m'\Gamma_{20}$

TABLE I: Representation matrices of selected generators of the little group at P in space group No. 230. The four matrices in the gray cells are obtained from Bilbao website and the rest are worked out by commutation relations.

We need to find the representation matrix for $\mathcal{PT}$ which is not given by Bilbao. We expand the 4D unitary U matrix by the 16 Gamma matrices with complex coefficients and determine the coefficients by the commutation relations in Table II.

	$\mathcal{PT} = U \cdot \mathcal{K}$		C_{2z}	C_{2y}	G	C_3
$\mathcal{PT}$	$\mathcal{PT}^2 = 1$	$UU^\dagger = 1$	$[C_{2z}, \mathcal{PT}] = 0$	$[C_{2y}, \mathcal{PT}] = 0$	$G(\mathcal{PT}) = i(\mathcal{PT})G$	$[C_3, \mathcal{PT}] = 0$

TABLE II: Compatibility relations used to determine $\mathcal{PT}$.

The sixteen Gamma matrices are $\Gamma_{ij} = \sigma_i \otimes \sigma_j$, ($i, j = 0, 1, 2, 3$), where $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, and $\otimes$ is the Kronecker product.

The Hamiltonian can be written as $H(\mathbf{k}) = A(k_x p_x + k_y p_y + k_z p_z)$, where k_x , k_y , k_z are three real variables (the origin is set at P in below), and p_x , p_y , p_z are three Hermitian matrices. To find p_x , p_y , p_z , we expand them as

linear combinations of 16 Gamma matrices with real coefficients and determine the coefficient by the commutation relations in Table. III.

For any representation matrix $D(g)$ of symmetry operation g (including $\mathcal{PT}$) in the little group, we have

$$D(g)H(\mathbf{k})D^{-1}(g) = H(g\mathbf{k}) \quad (1)$$

that gives the following commutation ($[\]=0$) and anti-commutation ($\{\}=0$) relations, listed in Table. III.

	p_z	p_y	p_x
$\mathcal{PT}$	$[\mathcal{PT}, p_z] = 0$	$[\mathcal{PT}, p_y] = 0$	$[\mathcal{PT}, p_x] = 0$
C_{2z}	$[C_{2z}, p_z] = 0$	$\{C_{2z}, p_y\} = 0$	$\{C_{2z}, p_x\} = 0$
C_{2y}	$\{C_{2y}, p_z\} = 0$	$[C_{2y}, p_y] = 0$	$\{C_{2y}, p_x\} = 0$
G	$[G, p_z] = 0$	$Gp_y = p_x G$	
C_3	$p_y = C_3^{-1} p_z C_3, p_x = C_3 p_z C_3^{-1}$		

TABLE III: Compatibility relations used to determine $H(\mathbf{k})$.

By satisfying all the requirements in Table. III, for Bilbao Rep. we obtain $p_z = \Gamma_{13} + w\Gamma_{23}$, ($w \in \mathbb{R}$). p_x and p_y are obtained from p_z by C_3 symmetry. Ignore the constant term A , the effective Hamiltonian is given as

$$H_D(\mathbf{k}) \sim (\sigma_x + w\sigma_y) \otimes (k_z\sigma_z + k_x\sigma_y - k_y\sigma_x) \quad (2)$$

After an unitary transformation, we get the representation matrix under Dirac Rep.

$$H_D(\mathbf{k}) \sim \sqrt{1+w^2} \begin{pmatrix} \mathbf{k} \cdot \boldsymbol{\sigma} & 0 \\ 0 & -\mathbf{k} \cdot \boldsymbol{\sigma} \end{pmatrix} \quad (3)$$

where $w \in \mathbb{R}$ is the velocity term. Note that the Dirac Hamiltonian we obtained above satisfies the exact massless Dirac equation in 3D. What listed in the last row of Table. I are the matrix of the Dirac mass terms, in corresponding basis with coefficients $m, m' \in \mathbb{R}$.

For space group No. 206, the only missing generator is $G = \{M|(-\frac{3}{4}, -\frac{3}{4}, \frac{1}{4})\}$ in $[1\bar{1}0]$ plane, and the Dirac Hamiltonian under Bilbao Rep. is

$$H_D(\mathbf{k}) \sim (\sigma_x + w\sigma_y + u\sigma_z) \otimes (k_z\sigma_z - k_x\sigma_x - k_y\sigma_y), \quad (w, u \in \mathbb{R}) \quad (4)$$

After an unitary transformation, we have the representation matrix under Dirac Rep.

$$H_D(\mathbf{k}) \sim \sqrt{1+w^2+u^2} \begin{pmatrix} \mathbf{k} \cdot \boldsymbol{\sigma} & 0 \\ 0 & -\mathbf{k} \cdot \boldsymbol{\sigma} \end{pmatrix} \quad (5)$$

III. DIRAC POINT UNDER SYMMETRY BREAKINGS

Dirac point lies in the phase transition center of many topological band nodal structures. In Table. IV we list the possible four bands nodal structures that can be achieved from perturbing the Dirac point, and list the corresponding key symmetries that need to be preserved($\checkmark$) or broken($\times$).

	Z_2 Dirac point	Z_2 nodal ring	Z_2 Weyl dipole	gapped Dirac	gapped	Weyl points	nodal ring
Z_2	1			0			
Realization	Fig. S2(a)	Fig. S2(b)	Fig. S2(c)	-	-	-	-
ω k							
Space group	No. 230	No. 088	No. 120	No. 220	-	-	-
	No. 206	No. 015	No. 045	No. 199	-	-	-
$\mathcal{PT}$	$\checkmark$	$\checkmark$	$\times$	$\times$	$\times$	$\times$	$\checkmark$
$G_i\mathcal{T}$	$\checkmark$	$\checkmark$	$\times$	$\times$	$\times$	$\times$	$\times$
$G_{j,k}\mathcal{T}$	$\checkmark$	$\times$	$\checkmark$	$\times$	$\times$	$\times$	$\times$
C_3	$\checkmark$	$\times$	$\times$	$\checkmark$	$\times$	$\times$	$\times$
l_0, l_1, l_2	0, 0, 0	$l_0, 0, 0$	$0, l_1, 0$	$0, 0, l_2$	$0, l_1 < l_2 $	$0, l_1 > l_2 $	-
Hamiltonian	$H(\mathbf{k}) \sim H_D(\mathbf{k}) + l_0\Gamma_{13} + l_1\Gamma_{03} + l_2\Gamma_{30}, (l_0, l_1, l_2 \in \mathbb{R})$ $H_D(\mathbf{k}) \sim (\sigma_x + w\sigma_y) \otimes (k_z\sigma_z + k_x\sigma_y - k_y\sigma_x)$						

TABLE IV: Possible results of the Dirac point transition under symmetry breaking.

IV. REALIZATION OF VARIOUS SYMMETRY BREAKINGS

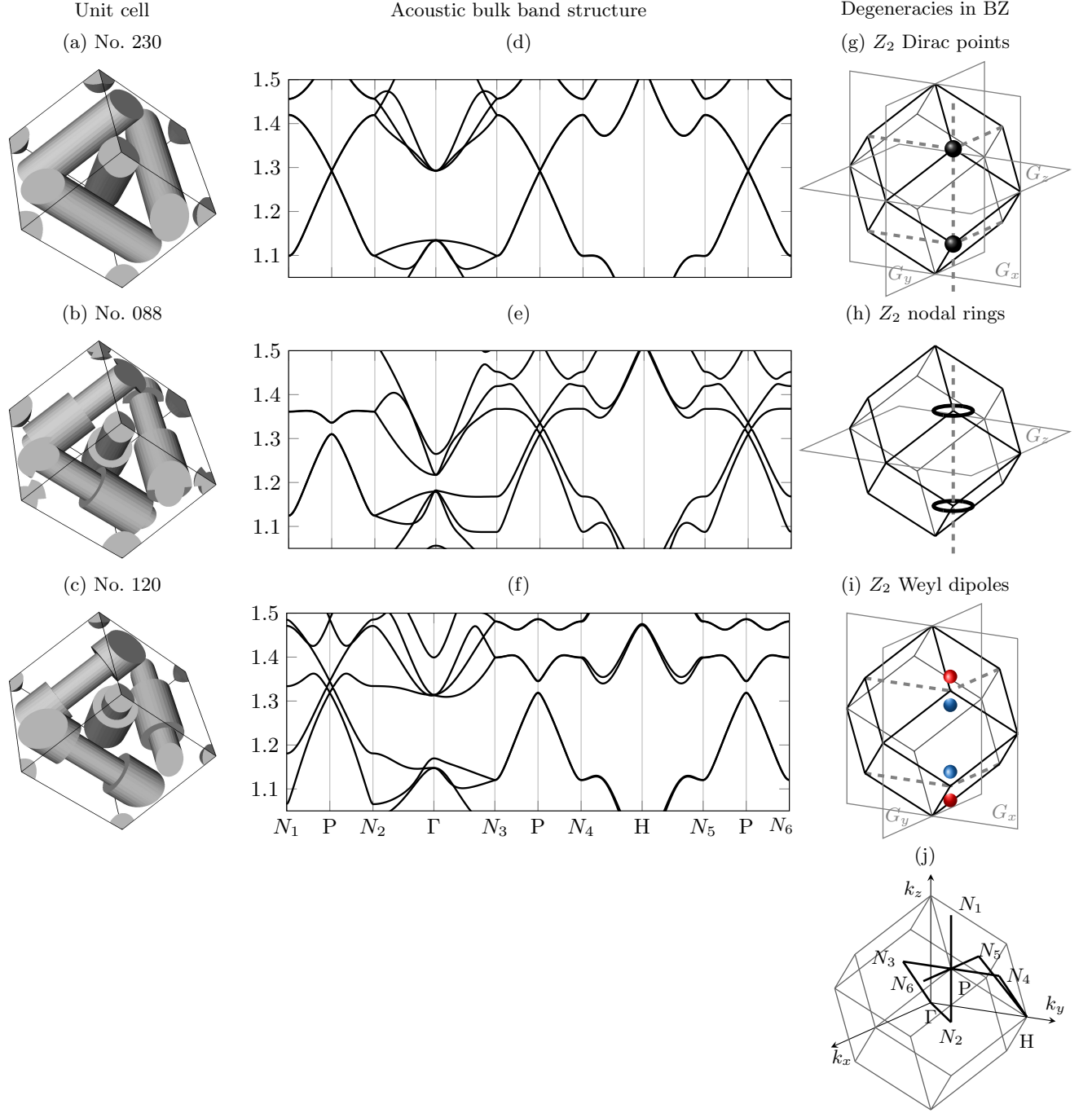


FIG. S2: Realization of the predicted symmetry breaking results. (a), (d), (g) Two Dirac points (black spheres) in the first BZ, locate at point $\pm P$. The dashed gray lines denote for the $G_i\mathcal{T}$ stabilized line degeneracies. (b), (e), (h) The Dirac points turn into Z_2 nodal rings (black circle). The $G_z\mathcal{T}$ stabilized degenerate lines, between lower or higher two bands, perpendicularly cross the rings and form nodal links within the four bands. (c),(f),(i) The Dirac points split into Z_2 Weyl dipoles (blue and red spheres for opposite chiralities). Since the two surface glides are not broken, the quad-helicoid surface states are still robust. Note that each one of $G_x\mathcal{T}$, $G_y\mathcal{T}$ is enough for keeping the Z_2 Weyl dipoles, but we need both to keep the quad-helicoid on 001 surface.

V. COMPARISON OF EIGENVALUE AND LDOS CALCULATIONS

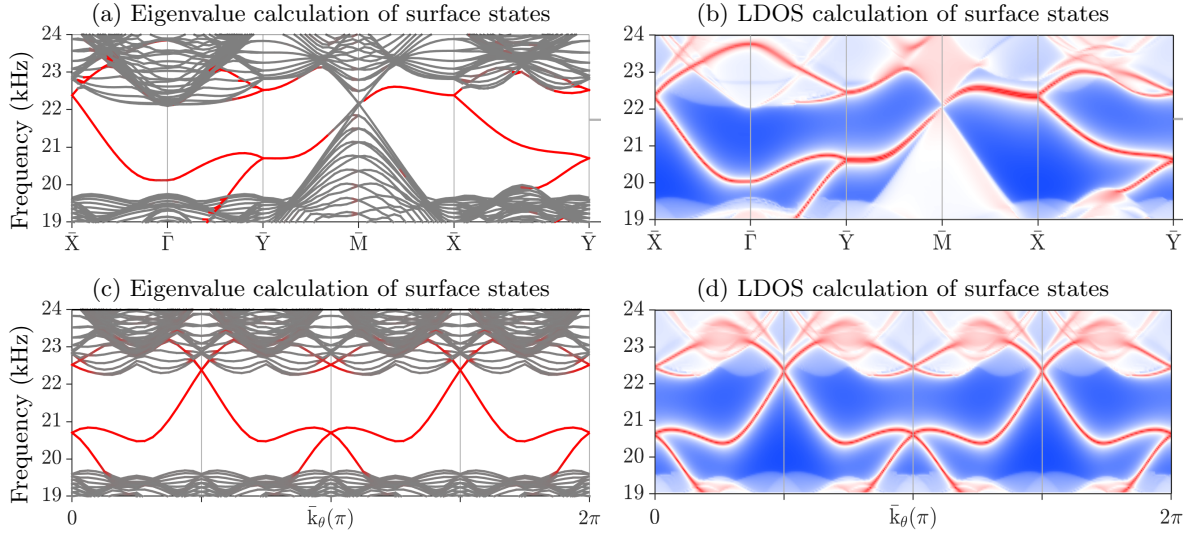


FIG. S3: Surface states in eigenvalue solutions and LDOS results. (a),(c) The surface states dispersion are obtained by solving the eigenvalue equation for a ten cubic cell stack with Floquet periodic boundary conditions in x and y directions and hard-wall boundaries on z and $-z$ ends. The dispersion lines were colored in red if they have a large energy fraction in the first two cells on the surface. The results agree the local density of states (LDOS) results in (b),(d), respectively.

VI. ADDITIONAL EXPERIMENTAL RESULTS

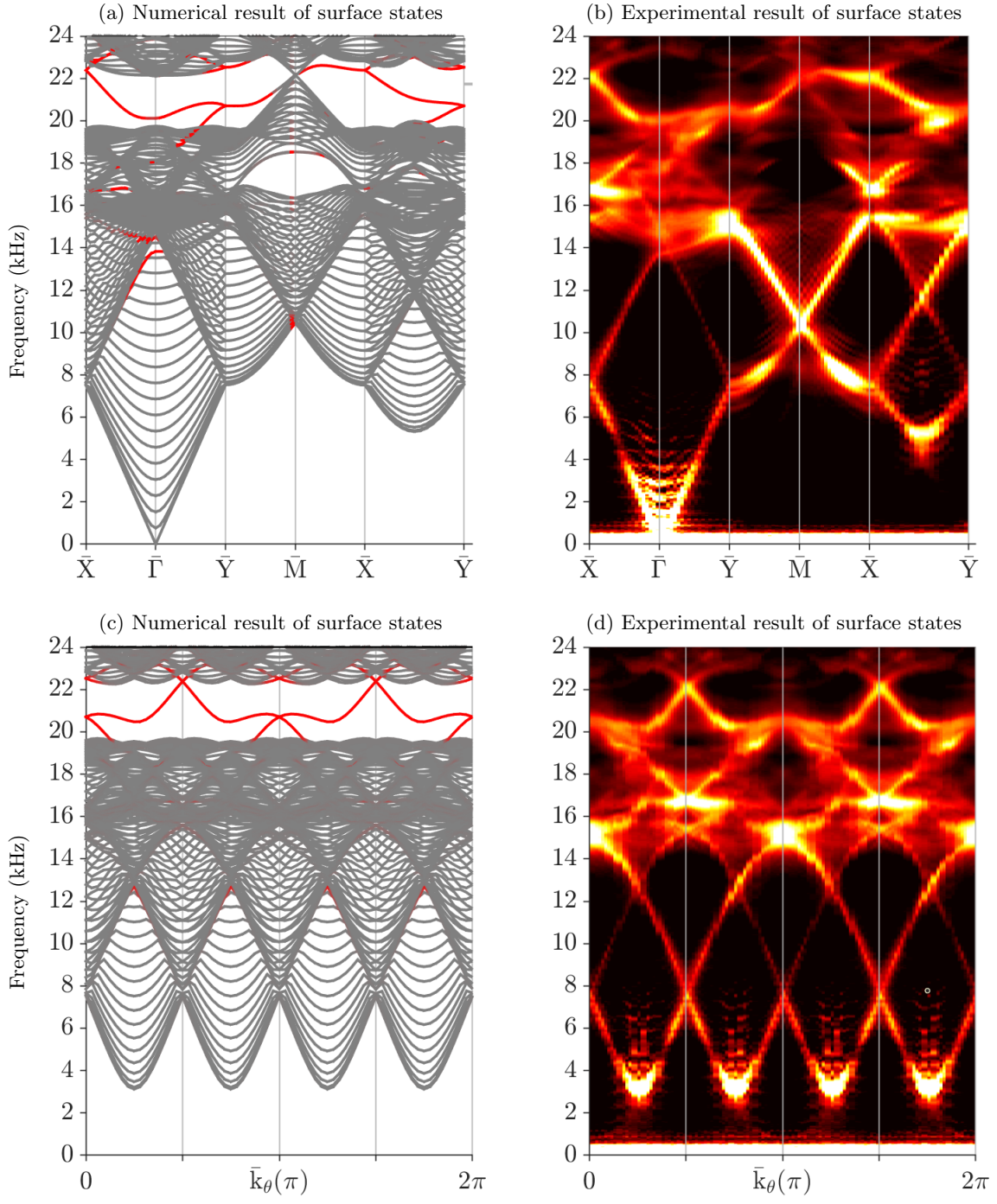


FIG. S4: Full frequency range data of the numerical and measured surface states.

VII. MORE DETAILS ON EXPERIMENTAL MEASUREMENTS

	Mass density ρ (kg/m^3)	Longitudinal sound velocity v_L (m/s)	Acoustic impedance $Z = \rho \cdot v_L$ ($N \cdot s/m^3$)
Air	1.2	343	412
Cured resin	~ 1140	~ 2240	$\sim 2.55e6$

TABLE V: Material properties of air and cured resin of 3D printing. Due to the 6200 times higher acoustic impedance of resin, the air-resin interface can be treated as hard-wall boundary conditions in calculations. The pressure field inside the resin are ignored.

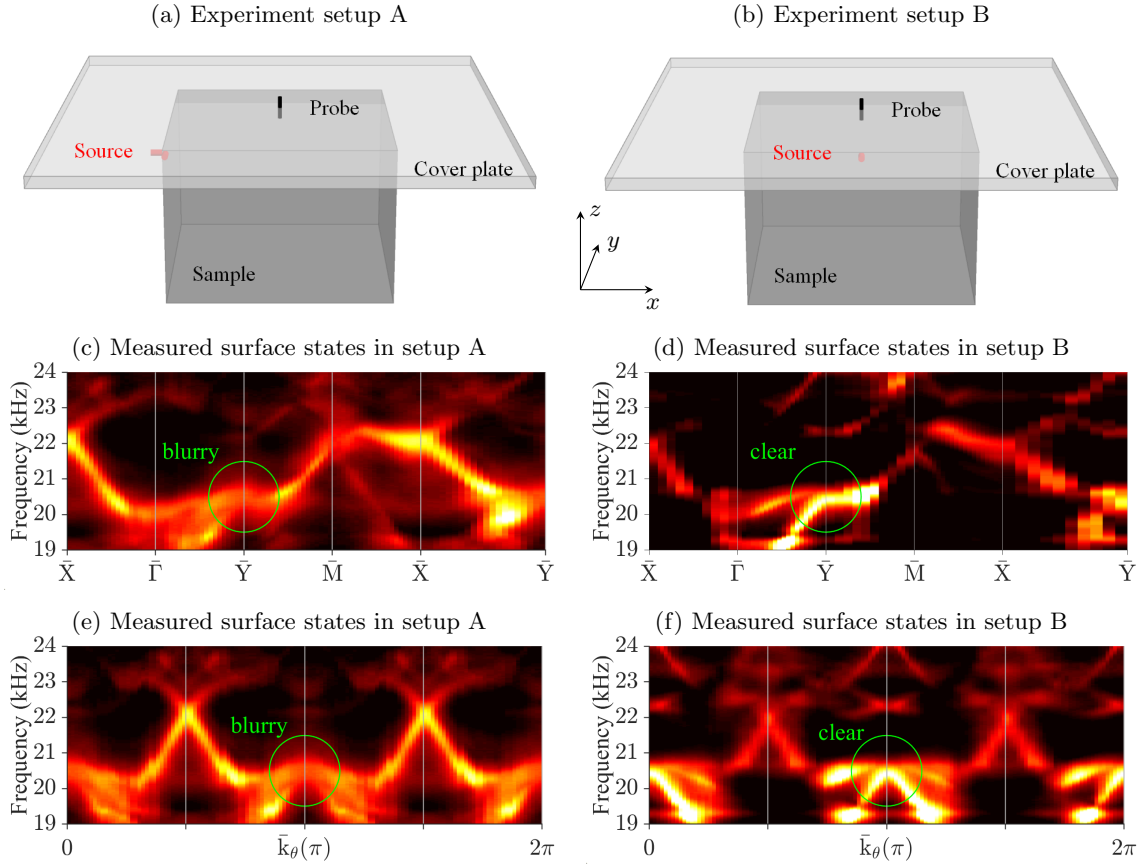


FIG. S5: Experimental data from different positions of the source excitations. (a) Setup A with the source fixed at the top corner of the sample, whose measurement results are shown in (c) and (e). (b) Setup B with the source fixed at the center of top edge of the sample, whose measurement results are shown in (d) and (f).