Topological valley crystals in a hexagonal Su-Schrieffer-Heeger (SSH) quantum Hall states

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Progress on two-dimensional materials has shown that valleys, as energy extrema in a hexagonal first Brillouin zone, provides a new degree of freedom for information manipulation. Then valley Hall topological insulators supporting such-polarized edge states on boundaries were set up accordingly. In this paper, a two-dimensional valley photonic crystal composed of six tunable dielectric triangular pillars in unit cells is proposed in the photonic sense of a deformed Su-Schrieffer-Heeger (SSH) model. We reveal the vortex nature of valley states and establish the selection rules for valley polarized states. Based on the valley topology, a rhombus-shaped beam splitter waveguide is designed to verify the valley-chirality selection above. Our numerical results entail that this topologically protected edge states still maintain robust transmission at sharp corners, henceforth providing a feasible idea for valley photonic devices in THz regime.

I. INTRODUCTION

In the past few years, inspired by the development of topological states of matter in condensed matter physics, such as quantum Hall states and topological insulator, the concept of topological band was introduced into valley photonic crystals (VPC) and quickly became a newly-chartered field. As the wave functions in photonic crystals (PC) appear similarly to that of electrons in solid physical systems, various phenomena originally discovered in condensed matter physics, such as quantum Hall, quantum spin Hall and quantum valley Hall effect, can be mapped to wave systems in analogue. As a pioneering work, F. Haldane and S. Raghunathan broke the time-reversal symmetry by applying an external magnetic field to the magneto-optical material, and proposed the photonic quantum Hall effect in the PC for the first time. Following the realization of the quantum Hall state using PC, photonic systems to simulate the quantum spin Hall effect using polarization degeneracy between transverse electric (TE) and transverse magnetic (TM) modes had been extensively studied. Recently, L.-H. Wu and X. Hu had successfully constructed a pair of pseudo-spin photonic states based on inequivalent irreducible representations of the $C_6$ symmetry group, by exploiting the TM mode and the fundamental crystal symmetry of an two-dimensional (2D) all-dielectric PC. This profound proposal was verified experimentally both in microwave and optical regimes.

Later on, a new degree of freedom (DOF) from the valley point, was also introduced to the PC platform. Valley points generally emerge at high-symmetry points of the Brillouin zone, and refer to local minima in the conduction band or local maxima in the valence band. The promise of using the valley DOF to store and carry information led to the conceptual breakthrough known as valleytronics in electronic applications generally. It was proposed that if the degeneracy between the two valleys is lifted, 2D materials could exhibit the quantum valley Hall effect, which is manifested by a pair of counter-propagating edge states with opposite valley-polarizations at non-trivial domain walls in the absence of scattering. The valley boundary state can be realized by combining two photonic crystals with different valley Chern numbers, i.e. the valley Hall PC. Valley Hall photonic crystals have been experimentally demonstrated at various frequencies and have found potential applications in topologically protected refractive high-efficiency waveguides, topological waveguide splitters, etc. To note, our model is a 2D variant of photonic Su-Schrieffer-Heeger (SSH) model when we adopt the hexagonal unit cell as shown below.

In this paper, we propose a two-dimensional VPC in SSH model whose unit cell is composed of six tunable dielectric triangular pillars, which makes use of reduced symmetry to switch topological phases. First, we propose a topological PC with Dirac points at valley points ($K/K'$) from its band structures. To verify the topological phase transition, we open the energy gap in the energy band at valleys by breaking the spatial inversion symmetry. By changing the intra/inter-cell coupling strengths, the degeneracy at the Dirac points can be lifted to result in a bandgap. Meanwhile, the Berry curvature in the reciprocal space is calculated to show a pair of energy extrema with different signs at the $K/K'$ point. The topological invariant (i.e., the valley Chern number) of VPCs is calculated by integrating the Berry curvature over the half Brillouin zone. Also, we demonstrate that with the valley excited states of our structure, the valley selectivity of PCs is revealed.

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by performing Fourier transform to their wave functions. Finally, we design a beam splitter of rhombus shape to verify the valley-selective transmission. Our work then provides a new idea for THz photonic devices manipulating valley DOF.

II. NUMERIC MODEL

In this paper, we consider a 2D hexagonal PC with \( C_6 \) symmetry, as shown in Fig. 1(a), the unit cell of which is composed of six dielectric pillars embedded in air.\(^{23,24}\) And the maximal Wyckoff points in the unit cell are represented by labels \( o,p,q \) in real space. The relative permittivity of the dielectric column is \( \varepsilon_d = 11.7 \). The lattice constant is \( a_0 = 50 \) \( \mu \)m, \( a_1 \) and \( a_2 \) are the lattice vectors. The dielectric pillars are equilateral triangles with the side length of \( r = a_0/4.9 \), and the distance from the center of the lattice to the center of the dielectric column is \( R_1 = R_2 = 19.7 \) \( \mu \)m \((R_1+R_2 = 39.4 \) \( \mu \)m\). We only consider the TM modes and all our results are calculated by a finite element method. The first Brillouin zone (FBZ) in the lattice contains a pair of \( K \) and \( K' \) points in its vertices, which are called valley points, as shown in Fig. 1(c) and its inset, where panel (c) displays the band structure of PC0. We use \( \Delta R = R_1-R_2 \) to stand for the intra/inter-cell couplings strength.\(^{25} \)

When \( \Delta R = 0 \), two degeneracy points appear at \( K/K' \) point with \( f = 2.37 \) THz due to the \( C_6 \) symmetry. By changing \( \Delta R \), the intra/inter-cell coupling change, and the lattice symmetry is reduced to \( C_3 \), and the degeneracy at the \( K/K' \) point is lifted, which is shown in Fig. 1(b) and (d). To be specific, the bandgap is opened in the frequency range of 2.2-2.35 THz when \( \Delta R = -6.4 \) \( \mu \)m. For another case, PC2 is constructed by changing \( \Delta R = R_1-R_2 = 6.4 \) \( \mu \)m, the corresponding band structure is shown in Fig. 1(d). The degeneracy points at \( K/K' \) are also lifted, and the bandgap appears from \( f = 2.2 \) THz to \( f = 2.35 \) THz. We symbol the lower and higher frequency state at \( K/K' \) as represented by \( K_1/K_1' \) and \( K_2/K_2' \) in panels (b) and (d). The valley states in gap exhibit chirality, which is manifest by the phase distribution of \( E_z \), i.e., arg \( E_z \). When \( \Delta R = -6.4 \) \( \mu \)m for valley \( K \), the phases of \( K_1 \) and \( K_2 \) have opposite vortex chirality at the position of \( p \) and \( q \), and vice versa for \( K' \) valley. PC2 has the opposite chirality to PC1 at \( K/K' \), indicating a typical band inversion that leads to a topological phase transition. Fig. 1(e) shows the width of the bandgap corresponding to different \( \Delta R \) sizes. The evolution of the unit cell when varying \( \Delta R \) is visualized in the Fig. 1(e) inset. When \( \Delta R \) changing from \( \Delta R = -6.4 \) \( \mu \)m to \( \Delta R = 6.4 \) \( \mu \)m, the closing and reopening of the bandgap occur. PC1 corresponding to \( \Delta R = -6.4 \) \( \mu \)m, PC0 corresponding to \( \Delta R = 0 \) \( \mu \)m, PC2 corresponding to \( \Delta R = 6.4 \) \( \mu \)m.

Then we focus on the properties of the \( K \)-valley state. The top and bottom panels in Fig. 2 represent the phase and amplitude distribution for the periodic lattice, which exhibit the chirality property of valley states. Therein, at the positions of high symmetry, \( p \) and \( q \) (i.e., threefold rotational symmetry \( C_3 \)), \( |E_z| \) vanishes and the phase becomes singular for both \( K_1 \) and \( K_2 \) valleys. The black arrows in the lower panel represent time-averaged Poynting vectors \( \mathbf{S} = \Re(\mathbf{E} \times \mathbf{H}^\ast)/2 \), which reveals a typical feature of a vortex field. Therefore, we can control the chirality of the valley vortex by switching the source chirality induced from positioning the dielectric pillars.\(^{26,27,28,29}\)

We then verify the valley selectivity\(^{30} \) of the structure in Fig. 3. Therein a chiral source with \( m = \pm 1 \) is placed at the center of the eddy current in the \( K/K' \) state, of which \( m \) is the vortex index of the field \( E_z \). And the excited electric field \( E_z \) distribution is shown in the left panel of Fig. 3. The spatial Fourier spectrum is plotted in the right panel of Fig. 3 where the green solid hexagons represent the Fourier Brillouin zone. These results show that \( K' \) state is excited when the source goes \( m = -1 \), and the \( K \) state is excited when \( m = +1 \).

By changing \( \Delta R \) and its inset, where panel (c) displays the band structure of PC0, \( \Delta R = 6.4 \) \( \mu \)m, \( \lambda_{\delta} \) and \( \epsilon \) are Pauli matrices acting on sublattice and valley spaces, respectively. \( \lambda_{\delta}^p \) indicates a frequency band gap due to the inversion asymmetry. And \( \lambda_{\delta}^p \approx [\int \rho \epsilon_z \, ds - \int \delta \epsilon_z \, ds] \) denotes the integration of \( \epsilon_z \) at the Blue(B) or Red(R) dielectric rods domains. In Fig. 4, a PC was shown in the figure, and the dashed rhomboid denotes a unit cell of PC. When \( \Delta R = -6.4 \) \( \mu \)m, as shown in Fig. 4(b), \( \int_0^\pi \epsilon_z \, ds < \int_\pi \epsilon_z \, ds \) leads to \( \lambda_{\delta}^p \approx 0 \) and a complete band gap appears and vice versa in Fig. 4(d). In Fig. 4(c), \( \Delta R = 0 \) \( \mu \)m, \( \int_0^\pi \epsilon_z \, ds < \int_\pi \epsilon_z \, ds \) and the band gap disappear with a degeneracy point is located in \( K/K' \) points. Moreover, the effective Hamiltonian implies a valley-dependent topological index of Berry curvature. The Berry connection of the lowest band can be defined as

\[
\vec{A}(\mathbf{k}) \equiv i \langle u_k | \nabla_k | u_k \rangle = i \oint_{\text{unitcell}} d^2 \mathbf{r} \epsilon(\mathbf{r}) u_k^* (\nabla_k u_k),
\]

where \( u_k \) is the electromagnetic fields, an asterisk denotes complex conjugation, and \( \epsilon(\mathbf{r}) \) is the spatial permittivity. And Berry curvature \( \Omega(\mathbf{k}) \) can be obtained from

\[
\Omega(\mathbf{k}) \equiv \nabla_k \times \vec{A}(\mathbf{k}) = \frac{\partial A_x(\mathbf{k})}{\partial k_y} - \frac{\partial A_y(\mathbf{k})}{\partial k_x}.
\]

The topological features of VPCs are related with the Berry curvature in the FBZ. As shown in Fig. 5(b), Berry curvature shows opposite signs at the \( K/K' \) points. For PC1 Berry curvature distribution around \( K \) have negative value, and a positive value with the same amplitude at \( K' \). On the other hand, PC2 has reversed Berry curvature distribution compared with PC1. Therefore, the integration of Berry curvature over the whole FBZ is 0. Topological indices at \( K \) and \( K' \) valleys, defined as the integration of Berry curvature within half Brillouin zone (HBZ), can be calculated as:

\[
C_{K/K'} = \frac{1}{2\pi} \int_{\text{HBZ}} \Omega(\mathbf{k}) d^2 \mathbf{k} = \pm \frac{1}{2} \text{sgn}(\Delta R).
\]
FIG. 1. Band structures and topological phase transition. (a) Schematic diagram of a two-dimensional (2D) hexagonal lattice with translation vectors of \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \) where the three positions in the lattice are labelled by o, p, q. The lattice constant is \( a_0 \). Six dielectric pillars with side length of \( r \) are placed in the lattice. (b),(c),(d) The band structure for the PC with \( \Delta R = R_1 - R_2 = -6.4 \, \mu \text{m}, 0 \, \mu \text{m}, 6.4 \, \mu \text{m} \) (insets of (b, d) shows the phase distributions). The lower and higher frequency state at \( K/K' \) are labelled by \( K_1/K_1' \) and \( K_2/K_2' \). (b) when \( \Delta R = -6.4 \, \mu \text{m}, \) at the \( p_1 \) and \( q_1 \) points the phase distributions reveal that \( K_1/K_1' \) and \( K_2/K_2' \) have opposite chirality, whose chirality is indicated by the black arrow in insets. (c) when \( \Delta R = 0 \, \mu \text{m}, \) the Dirac points appear at points \( K \) and \( K' \) in the FBZ, and the inset shows the FBZ of the lattice. (d) when \( \Delta R = 6.4 \, \mu \text{m}, \) \( K \) and \( K' \) valley points show opposite chirality compared to panel (b). (e) Frequency gap variation of PC lattice with change of \( \Delta R \) at Brillouin zone center \( K \) and the evolution of the unit cell is indicated in the inset.

The valley chern number is only determined by the sign of \( \Delta_p \). And the nonzero topological invariant, i.e., valley Chern number \( C_V = (C_K - C_{K'}) \) as depicted in Fig. 5(a), when \( \Delta R < 0, C_V = -1, \) and for \( \Delta R > 0, C_V = 1. \) Thus, PC1 and PC2 have quantized Chern number with opposite sign, which leads to a topological phase transition.

III. RESULTS AND DISCUSSION

Topological edge states at the zigzag interface: As the sign of the difference of the valley Chern numbers determines the propagation direction of the emerging edge states, this indicates that the edge state at one valley has a positive velocity whereas the other has a negative one, i.e., the valley-momentum locking behavior. To confirm this, as shown in Fig. 6(a), a \( 30 \times 1 \) cell structure composed of PC1 and PC2 is constructed in this paper. The separation interface is zigzag type, i.e. \( 30 \) cells in y-direction and infinite in x-direction. In simulation, Floquet periodic boundary conditions are imposed on the left and right boundaries of the supercell, and the upper and lower boundaries satisfy scattering boundary condition. The energy band for our valley crystal is shown in Fig. 6(c). The red line in figure represents the edge state with topological protection while the gray part represents the bulk band. It can be seen that the group velocities of the edge states at different valleys are opposite, indicating the valley-momentum locking behavior. Furthermore, Fig. 6(b) shows the spatial distribution of electric field with the frequency of \( 2.35 \) THz at \( k_x = \pm 0.35 \times 2\pi/a_0 \). Owing to the presence of finite valley Chern number, the localized EM states are observed along the interfaces. Since the topological kink states are locked within the \( K/K' \) valleys, inter-valley scattering is strongly suppressed despite the presence of obstacles of sharp corners. Such properties make the designed VPC an excellent candidate as waveguides.

Verification of valley-selective transmission: The valley-momentum locking edge states discussed above could be useful for designing functional EM devices, henceforth we designed a rhombus-shaped beamsplitter (shown in Fig. 6). The beamsplitter consists of four regions, which is selectively activated by the valley degree of freedom. The upper-left and lower-right areas are filled by PC1, and the lower-left and upper-right areas are filled by PC2. PC1/PC2 and PC2/PC1 domain walls are formed between different regions. We calculate the electric field in \( xy \) plane above the diamond waveguide to directly visualize the edge states and to analyze their valley polarization. The simulated electric fields are shown in Fig. 6(d) and (e), where the blue asterisk is the source and the white arrow the direction of the propagation edge state. At
FIG. 2. Electric field distribution $|E_z|$ of the K-valley state (low frequency $K_1$, high frequency $K_2$) at positions p, q. The upper and lower panels respectively represent the valley phase and electric field amplitude distribution of the periodic lattice, the arrows in the lower panel indicate the corresponding time-averaged Poynting vector.

FIG. 3. The electric field in $|E_z|$ stimulated by a chiral source with (a)$m = -1$ and (b)$m = 1$ positioned in the center of sample. The insets in the left panels represent the vortex feature of the chiral source. The right panels display the corresponding Fourier spectra in momentum space.

FIG. 4. Schematic diagram of a two-dimensional (2D) hexagonal lattice of dielectric rods embedded in an air background. e.g., blue and red rods in the dashed rhomboid. (b), (c) and (d) represent the unit cell with $\Delta R = -6.4 \ \mu m, 0 \ \mu m$ and $6.4 \ \mu m$.

FIG. 5. Distribution of valley Chern number. (a) The variation of valley Chern number with change of $\Delta R$. Blue dots for $C_v = -1$, red dots for $C_v = 1$, and the black line for the theoretical calculation. FBZ was shown in the inset. (b) Two PC structures and their corresponding Berry curvature distribution in the FBZ.

$f = 2.26 \ \text{THz}$, the edge state is successfully excited by the chiral source. The electric field is well confined along the interface and propagates only in the direction correlating with the chirality of the source.
IV. CONCLUSIONS

In conclusion, we design a VPC to reveal the dynamic process of topological phase transition by turning the inter/intra-cell coupling strength. In our design, a VPC based on $C_6$ symmetry is adopted with Dirac points at $K/K'$ points. And by positioning the dielectric columns in unit cells, the intra/inter couplings are adjusted leading to a reduced symmetry of $C_3$, when the degeneracy at Dirac points is lifted. Then two distinct valley states from our setup are demonstrated to verify the vortex feature of the wave function. Also we calculate the valley Chern number of the VPC accordingly and reveal the topological phase transition. Finally, we confirm the valley selection principle of the designed VPC in a beam splitter of rhombus shape. Our work then provides a new experimental setup for application of THz VPC devices.

Appendix A: More on the periodic unit lengths setup in numerics for supercells

In this Append., we plot three cases in Fig. 7 for dispersion bands of a VPC serving as building blocks of our beam splitter in Fig. 6.
FIG. 7. Three cases for dispersion bands of a VPC serving as building blocks of our beam splitter. Band structure of a (a) $30 \times 1$ (b) $30 \times 2$ (c) $30 \times 3$ supercell and the schematic of the supercell composed of PC1 and PC2 with zigzag interfaces is on the right of the dispersion bands.

FIG. 8. Simulated electric field distributions at (a) 2.22 THz, (b) 2.24 THz and (c) 2.26 THz on the xy plane with a chiral source at 1 port (lower panel) and 2 port (upper panel).

Appendix B: More field distribution on different work frequency of beam-splitters

In this Append., we simulate the electric field of the beam-splitter on more frequency. As seen in the Fig. 8, at $f = 2.22$ THz, 2.24 THz and 2.26 THz, the edge states are successfully excited by the chiral source.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

AUTHOR CONTRIBUTION

Z. Y. and H. L. proposed the idea. Z. Y. performed the calculation, produced all the figures, and wrote the manuscript draft. R. Z. contributed to the calculation tools. Z. Y. and Y. L. analyzed the data. H. L. and Y. L. lead the project and revised the whole manuscript thoroughly. Z. M. and K. P. contributed to analyzing the data and to revising the paper.

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