Topological Crystalline Insulators

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The recent discovery of topological insulators has revived interest in the band topology of insulators. In this work, we extend the topological classification of band structures to include certain crystal point group symmetry. We find a class of three-dimensional "topological crystalline insulators" which have metallic surface states with quadratic band degeneracy on high symmetry crystal surfaces. These topological crystalline insulators are the counterpart of topological insulators in materials without spin-orbit coupling. Their band structures are characterized by new topological invariants. We hope this work will enlarge the family of topological phases in band insulators and stimulate the search for them in real materials.

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The topology of band structures is important in the study of topological phases of matter. Historically the quantization of Hall conductance in the integer quantum Hall effect was explained by the Thouless-Kohmoto-Nightingale-den Nijs integer (also known as Chern number) of occupied bands[1]. Recently the topological classification of spin-orbital coupled band structures with time reversal symmetry has played a key role in the theoretical prediction of topological insulators[2–4]. The subsequent development of topological band theory[5], combined with realistic band structure calculations, has proven useful in the material search for topological insulators.

Inspired by the discovery of topological insulators, the classification of band structures has been extended to other discrete symmetry classes such as particle-hole symmetry[6–8], which leads to a rich family of topological phases such as topological superconductors[6, 9]. More recently, the classification of magnetic insulators with certain magnetic translation symmetry has been studied[10, 11]. Finding these phases in real materials is interesting and challenging.

The purpose of this work is to extend the classification of band structures in a different direction—to include crystal point group symmetries. We introduce the notion of "topological crystalline insulators", which cannot be smoothly connected to a trivial atomic insulator when time reversal (T) symmetry and certain point group symmetry are respected. Unlike time reversal symmetry, crystal symmetries can be broken by sample surfaces. As a result, a low-symmetry surface of a topological crystalline insulator does not have robust surface states. This motivates us to study a class of three-dimensional topological crystalline insulators which have four-fold (C_4) or six-fold (C_6) rotational symmetry. As we will show, its (001) surface, which preserves the rotational symmetry, supports gapless surface states. These topological crystalline insulators are the counterpart of topological insulators in materials *without spin-orbit coupling*. Instead electron's orbital degrees of freedom play a role similar to spin. Unlike topological insulators, the (001) surface states of topological crystalline insulators have *quadratic* band degeneracy protected by time reversal and discrete rotational symmetry[12, 13].

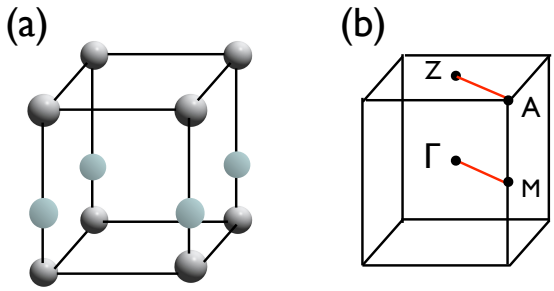

FIG. 1: (a) tetragonal lattice with two atoms A and B along the c-axis in the unit cell; (b) the Brillouin zone and four high symmetry points.

The outline of this paper is as follows. First we introduce a simple tight-binding model in a tetragonal crystal with C_4 symmetry. We explicitly show that gapless surface states exist on the (001) crystal face. The topological stability of surface states suggests a nontrivial phase in this model. Next we define a new Z_2 topological invariant for generic time reversal invariant band structures with C_4 or C_6 symmetry in three dimensions. This establishes the topological crystalline insulator phase. Finally we discuss the electronic properties of quadratic surface bands.

Tight-Binding Model: Consider a tetragonal lattice with a unit cell of two inequivalent atoms A and B along c-axis, as shown in Fig.1a. The 3D crystal can be viewed as a stack of bilayer square lattices in the ab plane. We now introduce a tight-binding model to describe the band structure of electron's p orbitals (or d orbitals, see the next paragraph). In particular, we are interested in the energy bands derived from p_x and p_y orbitals. We assume that these bands do not overlap with the p_z bands, and construct a tight-binding model from Wannier functions with the same symmetry as p_x and p_y orbitals. The Hamiltonian H consists of intra-layer hop-

ping H^A and H^B, as well as inter-layer hopping H^{AB}:

$$\begin{aligned} H &= \sum_n H_n^A + H_n^B + H_n^{AB}, \\ H_n^a &= \sum_{i,j} t^a(\mathbf{r}_i - \mathbf{r}_j) \sum_{\alpha,\beta} c_{a\alpha}^\dagger(\mathbf{r}_i, n) e_\alpha^{ij} e_\beta^{ij} c_{a\beta}(\mathbf{r}_j, n), \\ H_n^{AB} &= \sum_{i,j} t'(\mathbf{r}_i - \mathbf{r}_j)[\sum_\alpha c_{A\alpha}^\dagger(\mathbf{r}_i, n) c_{B\alpha}(\mathbf{r}_j, n) + h.c.] \\ &+ t'_z \sum_i \sum_\alpha [c_{A\alpha}^\dagger(\mathbf{r}_i, n) c_{B\alpha}(\mathbf{r}_i, n+1) + h.c.] \quad (1) \end{aligned}$$

Here each site is specified by $(n, \mathbf{r}, a)$: n labels the bi-layer unit cell along c-axis; $\mathbf{r} = (x, y)$ labels the ab-plane coordinate; $a = A, B$ labels the sublattice. α, β label the p_x, p_y orbital. Two types of p-orbital hopping terms appear in H. The intra-layer hopping in H^a is of σ-bonding type: it depends on the relative orientation of p-orbital and the hopping direction $\mathbf{e}^{ij} = (\mathbf{r}_i - \mathbf{r}_j)/|\mathbf{r}_i - \mathbf{r}_j|$. The inter-layer hopping in H^{AB} is orbital-independent. Written in this form, the tight-binding Hamiltonian manifestly preserves crystal symmetries. The hopping amplitudes t^a, t' and t'_z between two sites depend on their ab-plane distance $\mathbf{r}_i - \mathbf{r}_j$. Throughout this work, we assume spin-orbit coupling is negligible, so that electron's spin index is omitted.

We emphasize that the form of the Hamiltonian H is entirely determined by crystal symmetry. Because $d_{xz,yz}$ orbitals transform in the same way as $p_{x,y}$ orbitals under C_4, (1) also applies to materials with these d-orbital. Therefore (1) is potentially revelant to a large class of materials including transition metal compounds with t_{2g} orbitals near Fermi energy.

To obtain a minimal model for topological crystalline insulators, we include the nearest and next-nearest neighbor intra-layer hoppings in H^a with the amplitude t_1^a and t_2^a, as well as nearest and next-nearest neighbor inter-layer hoppings in H^{AB} with the amplitude t'_1 and t'_2. The corresponding Bloch Hamiltonian $H(\mathbf{k})$ is obtained by Fourier transform:

$$\begin{aligned} H(\mathbf{k}) &= \begin{pmatrix} H^A(\mathbf{k}) & H^{AB}(\mathbf{k}) \\ H^{AB\dagger}(\mathbf{k}) & H^B(\mathbf{k}) \end{pmatrix} \\ H^a(\mathbf{k}) &= 2t_1^a \begin{pmatrix} \cos k_x & 0 \\ 0 & \cos k_y \end{pmatrix} \\ &+ 2t_2^a \begin{pmatrix} \cos k_x \cos k_y & \sin k_x \sin k_y \\ \sin k_x \sin k_y & \cos k_x \cos k_y \end{pmatrix}, \\ H^{AB}(\mathbf{k}) &= [t'_1 + 2t'_2(\cos k_x + \cos k_y) + t'_z e^{ik_z}] I. \quad (2) \end{aligned}$$

The band structure is shown in Fig.2a for the following set of parameters: $t_1^A = -t_1^B = 1, t_2^A = -t_2^B = 0.5, t'_1 = 2.5, t'_2 = 0.5, t'_z = 2$. We have checked that the energy gap is finite everywhere in the Brillouin zone. As long as the energy gap does not close, the system remains in the same topological class within a finite parameter range.

To study surface states, we solve H in a slab geometry. We find that the existence of gapless surface states

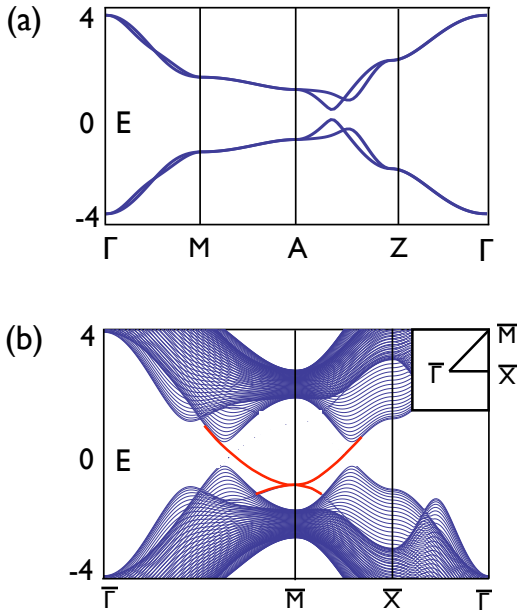

FIG. 2: (a) bulk band structure of the tight binding model along high symmetry lines; (b) surface states with quadratic band touching exist on (001) face. The tight-binding parameters are shown in the text below Eq.(2).

crucially depend on the surface termination. Consider the high symmetry (001) surface, which preserves the C_4 symmetry. Here surface states exist and transverse the whole energy gap as shown in Fig.2, leading to a 2D surface metal. Note that surface states are doubly degenerate at $\bar{M} = (\pi, \pi)$: one in p_x orbital and the other in p_y orbital. Because $\bar{M}$ is a fixed point under four-fold rotation, the doublet form a two-dimensional irreducible *real* representation of C_4 symmetry, as a result of time reversal symmetry for electrons without spin-orbit coupling (i.e., spinless fermions). Surface band dispersion near $\bar{M}$ can be obtained from $k \cdot p$ theory. We introduce a pseudospin $\sigma_z = \pm 1$ to label the p_x and p_y orbital of the doublet. In this basis, C_4 rotation is represented by $e^{i\sigma_y \pi/4}$ and time reversal operator T is represented by complex conjugation. Up to a gauge transformation, the form of the $k \cdot p$ Hamiltonian $\mathcal{H}$ is dictated by symmetry:

$$\mathcal{H}(k_x, k_y) = \frac{k^2}{2m_0} + \frac{k_x^2 - k_y^2}{2m_1}\sigma_z + \frac{k_x k_y}{2m_2}\sigma_x. \quad (3)$$

Perturbations which break either C_4 or T symmetry can open up an energy gap and destroy the protected surface states. This can be seen explicitly by adding a C_4-breaking term $M_1 k_x \sigma_y + M_2 \sigma_z$ or a T-breaking term $M\sigma_y$ to $\mathcal{H}$. Similar quadratic bands have been recently studied in 2D photonic crystals[12] and fermion models[13].

Our tight-binding model does not have gapless surface states for other surface terminations which break the C_4 symmetry.

When T and C_4 symmetry are preserved, the surface states shown above are *topologically* protected. This can be understood by considering the surface band dispersion along $\bar{\Gamma}\bar{M}$. Within our model, surface states (if present) must be doubly degenerate at $\bar{\Gamma}$ and $\bar{M}$. As a consequence, there exists two distinct types of surface band connectivity along $\bar{\Gamma}\bar{M}$, having an even or odd number of band crossings at Fermi energy respectively. Surface states with even crossings are fragile: they can be pushed out of the energy gap by changing the surface potential. Surface states with odd crossings have a Fermi surface which encloses $\bar{\Gamma}$ an odd number of times. They cannot be removed. These two types of surface states imply the existence of two topologically distinct phases of time-reversal-invariant band insulators with four-fold symmetry. The reasoning here closely follows the previous study of topological insulators[14].

Z_2 **Topological Invariant**: We now show that a Z_2 topological invariant $\nu_0 = 0, 1$ characterizes the band structure of 3D time-reversal-invariant insulators with four-fold rotation symmetry (without spin-orbit coupling). $\nu_0 = 0$ corresponds to a trivial phase adiabatically connected to an atomic insulator. $\nu_0 = 1$ corresponds to a topological crystalline insulator which has gapless surface states on the (001) surface.

We start by examining the symmetry property of Bloch wavefunctions of occupied bands: $|\psi_n(\mathbf{k})\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u_n(\mathbf{k})\rangle$, where $|u_n(\mathbf{k})\rangle$ is the cell-periodic eigenstates of the Bloch Hamiltonian $H(\mathbf{k}) \equiv e^{-i\mathbf{k}\cdot\mathbf{r}}He^{i\mathbf{k}\cdot\mathbf{r}}$. Here the unit cell is chosen to be invariant under C_4 rotation around the z axis. $H(\mathbf{k})$ satisfies

$$\begin{aligned} H(k_x, k_y, k_z) &= UH(k_y, -k_x, k_z)U^{-1} \\ H(k_x, k_y, k_z) &= TH(-k_x, -k_y, -k_z)T^{-1}. \end{aligned} \quad (4)$$

Here the unitary operator $U = e^{i\hat{L}_z\pi/2}$ implements C_4 rotation within the unit cell ($\hat{L}_z$ is angular momentum operator). The anti-unitary operator $T = K$ (complex conjugation) implements time reversal transformation for *spinless* fermions, with the property $T^2 = 1$. As a result, time reversal symmetry by itself does not guarantee a two-fold degeneracy. However, the combination of time reversal and four-fold rotational symmetry can lead to protected degeneracies at four special momenta $\Gamma = (0, 0, 0), M = (\pi, \pi, 0), A = (\pi, \pi, \pi), Z = (0, 0, \pi)$ in the 3D Brillouin zone (Fig.1b). At such a high symmetry point $\mathbf{k}_i$, $H(\mathbf{k}_i)$ commutes with U, so that the energy bands $|u_n(\mathbf{k}_i)\rangle$ are eigenstates of four-fold rotation with possible eigenvalues $1, -1, i$ and $-i$. Moreover, because $H(\mathbf{k}_i)$ is real, energy bands at $\mathbf{k}_i$ with $\pm i$ eigenvalues are guaranteed to be degenerate, forming a two-dimensional *irreducible real* representation of C_4. For example, such doublet bands can derive from (p_x, p_y) orbitals or (d_{xz}, d_{yz}) orbitals. From now on, we consider a set of energy bands $|u_n(\mathbf{k})\rangle, n = 1, ...2N$ which are doubly degenerate $E_{2n-1}(\mathbf{k}_i) = E_{2n}(\mathbf{k}_i)$ at Γ, M, A and Z. As we will see below, only these doublet bands admit a Z_2 classification.

The Z_2 topological invariant ν is defined in terms of the electron wavefunctions:

$$(-1)^{\nu_0} = (-1)^{\nu_{\Gamma M}}(-1)^{\nu_{AZ}}, \quad (5)$$

$$(-1)^{\nu_{\mathbf{k}_1\mathbf{k}_2}} = \exp(i\int_{\mathbf{k}_1}^{\mathbf{k}_2} d\mathbf{k}\cdot\mathcal{A}_{\mathbf{k}})\frac{\mathrm{Pf}[w(\mathbf{k}_2)]}{\mathrm{Pf}[w(\mathbf{k}_1)]}, \quad (6)$$

$$\mathcal{A}_{\mathbf{k}} \equiv -i\sum_j \langle u_j(\mathbf{k})|\partial_{\mathbf{k}}|u_j(\mathbf{k})\rangle,$$

$$w_{mn}(\mathbf{k}_i) \equiv \langle u_m(\mathbf{k}_i)|UT|u_n(\mathbf{k}_i)\rangle.$$

$\mathcal{A}_{\mathbf{k}}$ is the $U(1)$ Berry connection. $w(\mathbf{k}_i)$ is an $U(2N)$ matrix, as seen from the the symmetry properties of $H(\mathbf{k}_i)$. We now specify the integration path in (6). For $\nu_{\Gamma M}$, the integral is along an arbitrary line connecting Γ and M which lies *within* the 2D plane $k_z = 0$ in the Brillouin zone as shown in Fig.1b. Likewise, the integration path for ν_{AZ} lies in the plane $k_z = \pi$.

Both $\mathcal{A}$ and w depend on the choice of basis $|u_j(\mathbf{k})\rangle$, but we now prove that $\nu_{\mathbf{k}_1\mathbf{k}_2}$ is gauge invariant. Two different basis $|\tilde{u}_n(\mathbf{k})\rangle$ and $|u_n(\mathbf{k})\rangle$ are related by a $U(2N)$ gauge transformation:

$$|\tilde{u}_n(\mathbf{k})\rangle = \mathcal{G}_{nm}(\mathbf{k})|u_m(\mathbf{k})\rangle,\ \mathcal{G} \in U(2N) \quad (7)$$

This leads to the corresponding gauge transformation of $\mathcal{A}$ and w:

$$\begin{aligned} \tilde{\mathcal{A}} &= \mathcal{A} - i\mathrm{Tr}[\mathcal{G}^{-1}\partial_{\mathbf{k}}\mathcal{G}] = \mathcal{A} - i\partial_{\mathbf{k}}\log(\det[\mathcal{G}]) \\ \tilde{w} &= \mathcal{G}^* w \mathcal{G}^\dagger \end{aligned} \quad (8)$$

Using the identity $\mathrm{Pf}[X^T MX] = \det[X]\mathrm{Pf}[M]$, it is straightforward to verify that $\tilde{\nu}_{\mathbf{k}_1\mathbf{k}_2} = \nu_{\mathbf{k}_1\mathbf{k}_2}$ is gauge invariant.

We now further show that $(-1)^{\nu_{\mathbf{k}_1\mathbf{k}_2}} = \pm 1$ is a Z_2 quantity. It follows from (4) that at the two 2D planes $k_z = 0$ and $k_z = \pi$, $H(\mathbf{k})$ has the symmetry property: $H(\mathbf{k}) = \Xi H(\mathbf{k})\Xi$, $\Xi \equiv U^2T$. This allows us to choose a *real* gauge along the integration path to evaluate (6):

$$\Xi|u_m(\mathbf{k})\rangle = -|u_m(\mathbf{k})\rangle, \quad (9)$$

Because Ξ is anti-unitary, $\mathcal{A} = 0$ everywhere along the integration path. So in this gauge $(-1)^{\nu[\mathbf{k}_1,\mathbf{k}_2]}$ reduces to

$$(-1)^{\nu_{\mathbf{k}_1\mathbf{k}_2}} = \mathrm{Pf}[w(\mathbf{k}_2)]/\mathrm{Pf}[w(\mathbf{k}_1)]. \quad (10)$$

Because $|u_m(\mathbf{k}_i)\rangle$ belong to the two-dimensional representation of C_4 group, we have $U^2|u_m(\mathbf{k}_i)\rangle = -|u_m(\mathbf{k}_i)\rangle$, so that the gauge condition (9) at $\mathbf{k}_i$ is equivalent to $T|u_m(\mathbf{k}_i)\rangle = |u_m(\mathbf{k}_i)\rangle$, i.e., the wavefunction is real. Under this reality condition, the matrix $w(\mathbf{k}_i)$ simplifies to

$$w_{mn}(\mathbf{k}_i) = \langle u_m(\mathbf{k}_i)|U|u_n(\mathbf{k}_i)\rangle. \quad (11)$$

Now by choosing a particular kind of real basis $|u_{2m}(\mathbf{k}_i)\rangle \equiv U|u_{2m-1}(\mathbf{k}_i)\rangle$, $w(\mathbf{k}_i)$ reduces to a standard form $w^0 = \epsilon \oplus \epsilon ... \oplus \epsilon$, which is a direct sum of N 2×2 Levi-Civita tensors. This means that in a generic real basis, $w(\mathbf{k}_i)$ can be written as

$$w(\mathbf{k}_i) = O^T(\mathbf{k}_i) w^0 O(\mathbf{k}_i),\ O(\mathbf{k}_i) \in O(2N). \qquad (12)$$

So we have

$$\mathrm{Pf}[w(\mathbf{k}_i)] = \det[O(\mathbf{k}_i)]\mathrm{Pf}[w^0] = \det[O(\mathbf{k}_i)] = \pm 1. \quad (13)$$

This proves that $(-1)^{\nu_{\mathbf{k}_1\mathbf{k}_2}} = \pm 1$ is a gauge invariant Z_2 quantity. So both $\nu_{\Gamma M}$ and ν_{AZ} are Z_2 topological invariants which characterize the band structures in the 2D momentum space $k_z = 0$ and $k_z = \pi$ respectively. Their product ν_0 is defined for 3D time-reversal-invariant insulators with C_4 symmetry, and determines the surface state property: gapless surface states exist on (001) face only when $\nu_0 = 1$. This is verified in the tight-binding model (1). The relation between ν_0 and $\nu_{\Gamma M}, \nu_{AZ}$ is analogous to that of strong and weak Z_2 index in 3D topological insulators[15–17].

Generalization to Crystals with C_6 Symmetry: The study of topological crystalline insulators with C_4 symmetry can be generalized to hexagonal crystal structures with C_6 symmetry. In that case, (001) surface states have quadratic degeneracy points either at $\bar{\Gamma}$ or two equivalent $\bar{K}$. The topological invariant is similarly defined by Eq.(6) from the electron wavefunctions on the lines ΓK and AH in the Brillouin zone. A concrete tight-binding model can be obtained by placing (1) in a layered triangular lattice. The details will be reported elsewhere.

The fact that the above Z_2 invariant is only defined for doublet bands illustrates the important interplay between symmetry representation and topology of energy bands in solids, a feature absent in other known classes of topological insulators. We are not aware of a systematic mathematical approach to classifying vector bundles (e.g., electron wavefunctions over the Brillouin zone) with given representations of group action (e.g., C_4 rotation) at fixed points (e.g. high symmetry momenta $\mathbf{k}_i$). We hope the concrete topological invariant (6) can stimulate continuing research on topological crystalline insulators with other lattice structures.

The occupied bands of real materials usually have both doubly degenerate and nondegenerate singlet components. Provided that the doublet bands are energetically separable from the singlet ones (i.e., no band crossing between them), the Z_2 invariant remains well-defined for the former. The coexistence with singlet bands can in principle weaken the stability of surface states[18], although this senario seems unlikely to happen in reality.

Surface States with Quadratic Degeneracy: Quadratic degeneracies in 2D band structure have attracted considerable interest recently. The $k\cdot p$ Hamiltonian (3) is widely used as a low energy approximation for the band structure of bilayer graphene near $\pm K$ points. However, unlike topological crystalline insulators, the quadratic degeneracy there is *not* protected by symmetry. Instead, the band dispersion very close to $\pm K$ becomes linear due to trigonal warping effects.

Electron interactions can drive 2D bands with quadratic degeneracy into a variety of interesting broken symmetry phases including quantum anomalous Hall state, nematic phase and etc[13]. The competition between different ordered phases is of great interest in bilayer graphene. It remains to see what happens in the *single-valley* quadratic surface states of topological crystalline insulators.

It would be interesting to generalize the concept of topological crystalline insulators to interacting systems. For example, crystal symmetry is known to play an important role in the topological classification of spin liquids[19], spin chains[20], and Mott insulators[21]. A unifying theory of symmetry protected topological phases remains to be developed.

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