Layer Construction of Topological Crystalline Insulator LaSbTe

Yuting Qian,1, 2, ∗ Zhiyun Tan,1, 3, ∗ Tan Zhang,1, 2 Jiacheng Gao,1, 2 Zhijun Wang,1, 2 Zhong Fang,1, 2 Chen Fang,1, 2, † and Hongming Weng1, 2, 4, †

1Beijing National Laboratory for Condensed Matter Physics,
 and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
2University of Chinese Academy of Sciences, Beijing 100049, China
3School of Physics and Electronic Science, Zunyi Normal University,
 Zunyi 563006, Guizhou, People’s Republic of China
4Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China

Topological crystalline insulator (TCI) is one of the symmetry-protected topological states. Any TCI can be deformed into a simple product state of several decoupled two-dimensional (2D) topologically nontrivial layers in its lattice respecting its crystalline symmetries, so called the layer construction (LC) limit. In this work, based on first-principles calculations we have revealed that both the tetragonal LaSbTe (∥LaSbTe) and the orthorhombic LaSbTe (∥LaSbTe) can be looked as a stacking of 2D topological insulators in each lattice space. The structural phase transition from ∥LaSbTe to ∥LaSbTe due to soft phonon modes demonstrates how the real space change can lead to the modification of topological states. Their symmetry-based indicators and topological invariants have been analyzed based on LC. We propose that LaSbTe is an ideal example perfectly demonstrating the LC paradigm, which bridges the crystal structures in real space to the band topology in momentum space.

Introduction.—Topological crystalline insulators (TCIs) [1] are topological states protected by crystalline symmetry as an extension of time-reversal (TR) symmetry protected topological insulators (TIs) [2–4]. It is known that three-dimensional (3D) weak TI protected by lattice translation can be obtained from stacking many copies of 2D TI in the third dimension. Heuristically, apart from translation, it has further been found that TCI protected by mirror symmetry can be adiabatically connected to the limit of weakly coupled 2D topology states. Initially, these 2D topological states were proposed to be 2D TCIs characterized by mirror Chern number [5] and 2D Chern insulators [6]. This has inspired people to grasp the physical picture of TCI from the perspective of “layer construction” (LC). Based on this, more general dimensional reduction arguments [7–10] were proposed which demonstrated that all crystalline point group symmetry-protected-topological phases can be produced by stacking lower-dimensional blocks of invertible topological states and the classification of these topological states obtained by this way are consistent with the results given by Thorngren et al. [11] for interacting bosons and Khatraf et al. [12] for free fermions. This provides us a clear understanding of the physical nature of the crystalline symmetry-protected topological phase.

Along this line, Song et al. [13] have further exploited the LC scheme and derived exhaustive mappings from symmetry data to topological invariants for arbitrary space groups in the presence of TR symmetry, which provides an effective approach to define and search for new TCIs [14–16] when combined with topological quantum chemistry (TQC) [17, 18] and symmetry-based indicators (SBI). LC decorates the lattice with 2D insulating layers with nontrivial $Z_2$ number or mirror Chern number, while atomic insulators are constituted from proper atomic orbitals at Wyckoff positions. But the correspondence between a LC and the resulted TCI is not as intuitive as the atomic picture. Recently, A. Matsugata et al. tried to connect the high-order TIs (HOTIs) to lower-dimensional TIs relying on tight-binding model to capture the essence of HOTIs [19], which gave a clear physical image. However, there is still no realistic TCI material with layered crystal structure to have exact one-to-one correspondence between the stacking of lower-dimensional topological phases in real space and the band topology.

In this paper, we introduce such a candidate – LaSbTe that has two distinct crystal structures: one is in tetragonal phase (∥LaSbTe) and the other is in orthorhombic phase (∥LaSbTe), of which t-LaSbTe is a member of WHM family [20]. When spin-orbit coupling (SOC) is taken into consideration, t-LaSbTe is a weak TI with one 2D TI in its unit cell while o-LaSbTe is a TCI with two 2D TI layers per unit cell due to the doubling of t-LaSbTe cell along the stacking direction in phase transition. Thus, o-LaSbTe can be viewed as a layer construction of two t-LaSbTe with proper lattice distortion, where each t-LaSbTe represents a layer of an elementary LC (eLC). To the best of our knowledge, this is the first system perfectly demonstrating the LC scheme, i.e., mapping the crystal structures in real space to the band topology in momentum space. This paves the way for understanding the physical essence of TCI.

Methodology.—The Vienna ab initio simulation package (VASP) [21, 22] with the projector augmented wave (PAW) method [23, 24] based on density functional theory was employed for the first-principles calculations. The generalized gradient approximation (GGA) of
Perdew-Burke-Ernzerhof type [25] was used for exchange-correlation potential. The cut-off energy for plane wave expansion was set 300 eV. The BZ was sampled as grids of $8 \times 8 \times 4$ for $t$-LaSbTe and $12 \times 12 \times 3$ for $\alpha$-LaSbTe in the self-consistent process, respectively. A width of 0.02 eV was adopted in the Gaussian smearing method for Fermi level determination. We employed the experimental lattice parameters [26, 27] and then fully relaxed the structure until the forces on all atoms were smaller than 0.01 eV/Å. The band structures were calculated with and without considering of spin-orbit coupling. The WannierTools [28] was employed to compute the surface states based on the maximally localized Wannier function (MLWF) constructed by Wannier90 [29]. The phonon spectrum was computed using Phonopy program based on the density functional perturbation theory (DFPT) [30]. The Wilson-loop technique was used to compute Time-Reversal $Z_2$ in single-layer calculation.

Crystal structure.—Two different crystal structures have been reported for LaSbTe. One is $t$-LaSbTe in a tetragonal phase with space group (SG.) $P4/nmm$ (No. 129). The relaxed lattice constants are $a = b = 4.421$ Å and $c = 9.659$ Å, being comparable with experimental values of $a = b = 4.44$ Å and $c = 9.47$ Å. La and Te are at Wyckoff position $2c$ (0.5, 0, 0, $z$) with $z = 0.7785$ and 0.1282, respectively. Sb is at $2b$ (0, 0, 0, 0.5). This is one of the $WHM$ family materials, [20] which can be looked as stacking of quintuple layers (QLs) along $c$-axis, where the QL is composed of five square nets in a sequence of [Te-La-Sb$_2$-La-Te] [31]. The QLs are bonded with each other along $c$-direction as indicated by the dotted lines in Fig. 1 (a) and they are suggested to be weaker than the bonds among square nets in QL.

The other one is $\alpha$-LaSbTe in orthorhombic phase with SG. $Pmnc$ (No. 62), the relaxed lattice constants are $a = 4.422$ Å, $b = 4.433$ Å and $c = 19.348$ Å. The experimental lattice constants are $a = 4.378$ Å, $b = 4.403$ Å and $c = 19.242$ Å. La, Te and Sb are at Wyckoff position $4c$ (0.2500, 0.2623, 0.6106), (0.2500, 0.2614, 0.4360) and (0.2500, 0.7283, 0.2491), respectively. Compared with $t$-LaSbTe, there are two QLs in one unit cell of $\alpha$-LaSbTe, which can be effectively looked as the dimerization of QLs since the square-sheet layer of Sb in each QL is distorted and the Sb sheets in neighboring QLs distort in opposite way. $\alpha$-LaSbTe has the inversion symmetry, a mirror plane ($m_{100}^{100}$), two glide planes ($g_{010}^{100}$, $g_{001}^{001}$) and three twofold screw axes ($g_{200}^{100}$$g_{010}^{001}$, $g_{100}^{001}$).

The structural difference in these two phases can be understood by studying their phonon spectra, which are calculated and shown in Fig. 2(a,b). The phonon spectrum of $\alpha$-LaSbTe indicates it is the stable phase, while that of $t$-LaSbTe has soft modes with imaginary frequencies at $\Gamma$ and $Z$. The soft modes at $Z$ (0, 0, 0.5) suggest that doubling of $c$-axis would lead to a dynamically stabilier crystal structure. These soft modes mainly consist of the Sb vibration modes as shown in Fig. 2(c), where the Sb atoms in neighboring QLs shift in opposite direction. This leads to a rectangular in-plane lattice and a zigzag chain like structure as schematically depicted from both top and side views in Fig. 2(d-f). Such kind of lattice distortion exactly corresponds to a structural transition.
from \(t\)-LaSbTe to \(o\)-LaSbTe. The soft modes at \(\Gamma\) are from optical phonon branches, which would result in a phase transition to crystal structure of SG. 11. Nonetheless, the transition to \(o\)-LaSbTe with SG. 62 happens in experiments while the phase of SG. 11 has not been reported.

**Electronic band structures.**—The band structures for \(t\)-LaSbTe and \(o\)-LaSbTe without and with SOC are shown in Fig. 3. It is known that as a family of WHM compounds, \(t\)-LaSbTe has nodal lines when SOC is neglected [20, 32]. This can be easily seen since there are band crossings along \(\Gamma-X(Y), \Gamma-M\) in \(k_z = 0\) plane and \(Z-R, Z-A\) in \(k_z = \pi\) plane. All the nodal lines are gapped when SOC is further included and \(t\)-LaSbTe becomes a weak TI as a simple stacking of QLs, i.e., 2D TIs [20]. There are also crossing points in band structure of \(o\)-LaSbTe without SOC, which are parts of the nodal lines in the mirror plane \(m_{100}^{100}\) as schematically shown in 1(f). Again, SOC will open band gap along the nodal lines and \(o\)-LaSbTe becomes a TCI.

According to the theory of SBI [16, 18], both \(t\)-LaSbTe and \(o\)-LaSbTe have inversion symmetry and their symmetry indicators are \(Z_{2,2,2,4}\) when SOC is considered, which can be easily calculated through Fu-Kane like formula [12, 13]. The three weak \(Z_2\) indices, denoted as \(z_{2w,i=1,2,3}\), are obtained through

\[
z_{2w,i=1,2,3} \equiv \sum_{\mathbf{K} \in \text{TRIM at } \{k_z = \pi\}} n^-_{\mathbf{K}} \mod 2. \tag{1}
\]

The \(Z_4\) indicator, denoted as \(z_4\) is from:

\[
z_4 \equiv \sum_{\mathbf{K} \in \text{TRIM}} \frac{n^+_{\mathbf{K}} - n^-_{\mathbf{K}}}{2} \mod 4, \tag{2}
\]

where the \(n^+_{\mathbf{K}} (n^-_{\mathbf{K}})\) is the number of occupied Kramer parity at time-reversal invariant momentum (TRIM) \(\mathbf{K}\). The number of occupied Kramer pairs with negative parity at eight TRIMs in the BZ has been marked in Fig. 1. Therefore, according to Eq. 1 and 2, we can get \(t\)-LaSbTe is a weak TI with \(Z_{2,2,2,4}\) being \((0010)\) and \(o\)-LaSbTe is a TCI of \((0002)\). It is known that each single layer, i.e., QL of \(t\)-LaSbTe is a 2D TI [20]. After phase transition, the distorted QL is still a 2D TI. The two QLs in one unit cell of \(o\)-LaSbTe are weakly coupled as a simple stacking. These differences and their corresponding topological invariants, as well as topological properties can be further understood through LC scheme, which relates the real space crystal structure with the band topology in momentum space.

**Layer Construction and Topological Invariants.**—Intuitively, \(t\)-LaSbTe can be looked as being constructed by putting a layer of 2D TI on the planes with Miller indices of \((001; \frac{1}{2})\). Applying all the symmetrical operations of SG. 129 on this layer gives out the same Miller planes. Therefore, eLC of \((001; \frac{1}{2})\) is shown in Fig. 1(b). It intersects \(a\)-axis and \(b\)-axis zero times and \(c\)-axis once per unit cell, leading to the three weak topological invariants \(Z_{2w,i=1,2,3}\) being 0, 0 and 1, respectively. The eLC of \((001; \frac{1}{2})\) occupies only four inversion centers out of eight, which means the topological invariant \(\delta_i\) protected by inversion symmetry for this eLC is convention-dependent and \(z_4 = 0, \delta_i = 0\). This eLC doesn’t occupy any rotation.
or screw axis, nor any mirror or glide plane. Further, it
doesn’t lead to nonzero stacking invariant for any screw
and glide symmetry. These mean the topological invariant
due to rotation, screw, mirror or glide symmetries are all zero, and thus \( t \)-LaSbTe is a weak TI instead of TCI.

The structural phase transition from \( t \)-LaSbTe to \( o \)-
LaSbTe has been revealed by the soft modes at \( Z \) of \( t \)
LaSbTe. This results in doubling of unit cell along \( c \)-axis and shifts of atoms. Therefore, there are two 2D TIs
decorating the lattice of \( o \)-LaSbTe in the Miller planes of
\((001; \frac{1}{2})\) and \((001; \frac{1}{4})\). These two Miller planes
decorated with 2D TIs constitute the eLC of \((001; \frac{1}{2})\) or
\((001; \frac{1}{4})\) within the lattice of SG. 62. In the convention
of choosing unit cell in this work, these two layers intersect all the three lattice vectors even times and
\( z_{\text{2ne,1,2,3}} = 0 \). All the inversion centers, as marked
in Fig. 1(e), are occupied by these two 2D TI layers, which
means \( \delta_i = 1 \) and \( z_4 = 2 \). Again, these two layers
are not in any mirror or glide plane, neither passing
through any rotation axis. However, they contribute
nonzero glide-stacking-number for glide symmetry \( g_{01}^{1012} \)
and nonzero screw-stacking-number for screw symmetries
\( s_{201}^{100} \) and \( s_{011}^{200} \). The corresponding topological hour-
glass invariant \( \delta_h \) and screw invariant \( \delta_s \) equal to one. In
this way, the topological state protected by time-reversal
and crystalline symmetries of \( o \)-LaSbTe has been fully
determined. It is a TCI with symmetry indicators of
\( z_{22224} = (0002) \) and topological invariants of \( \delta_i = 1, \)
\( \delta_h^{(010)} = 1 \) and \( \delta_s^{(100)} = \delta_s^{(001)} = 1 \).

Topological Surface States from Topological Invari-
ants.—The nonzero hourglass invariant \( \delta_h \) suggests that
there exists nontrivial hourglass SS on the surface that
preserves corresponding glide mirror symmetry \([33, 34]\).
It is known that the Wilson loop spectrum defining the
bundle of occupied states over the \( \text{BZ} \) is isomorphic to
the spectrum of SS \([35]\). One can check the hourglass
invariant by calculating either the spectrum of Wilson
loop based on bulk Hamiltonian, or the SS on the correspon-
ding surface based on surface Green’s function method
with truncated surface as boundary condition \([28, 36]\).
For the hourglass invariant \( \delta_h^{(010)} = 1 \), it will protect
the nontrivial hourglass SS along the paths \( \tilde{\Gamma} - \tilde{Z} \)
and \( \tilde{R} - \tilde{Y} \) on \((100)\)-surface as shown in Fig. 1(f) since
the glide plane \( g_{01}^{1012} \) is preserved and projected to them.
The Wilson loop spectra in Fig. 4(a) and (b) clearly show that
there are hourglass-like SSS along \( \tilde{\Gamma} - \tilde{Z} \) and \( \tilde{R} - \tilde{Y} \). And
the connecting curves \( \tilde{Z} - \tilde{R} \) between these two hour-
glasses with a generalized zigzag pattern exhibit a spec-
tral flow \([34]\). In the SS calculation within Green’s function
method, the hourglass-like SS along \( \tilde{\Gamma} - \tilde{Z} \) can be
clearly reproduced in Fig. 4(c). However, the one along
\( \tilde{R} - \tilde{Y} \) is hardly to be seen as mixed with the gapless bulk
states. Similarly, \( \delta_h^{(001)} \) is trivial and there should be no
topological SS when projected along \( \tilde{Z} - \tilde{R} \) and \( \tilde{Y} - \tilde{\Gamma} \) on
\((110)\)-surface, which keeps the glide symmetry \( g_{12}^{010} \). The
hourglass-like spectra along \( \tilde{Z} - \tilde{R} \) and \( \tilde{Y} - \tilde{\Gamma} \) shown in
Fig. 4(d, e) are actually trivial since the connection be-
tween them shows a spectrally isolated quadruplets with
a full gap when viewed along \( \tilde{Z} \tilde{R} \tilde{Y} \tilde{T} \) in whole surface \( \text{BZ} \),
which is consistent with the trivial topological SS band
structure in Fig. 4(f).

The nontrivial screw invariant \( \delta_s \) can lead to protected hinge states, which have been carefully discussed in sev-
eral works \([33, 37, 38]\) and will not be presented here for
simplicity.

Conclusion.—Based on the first-principles calculations,
we conclude that a TCI phase \( o \)-LaSbTe with
hourglass SS and hinge state can be viewed as stacking
of two \( t \)-LaSbTe due to structural phase transition.
This dimensional reduction method can effectively capture
the physics of TCI. Specially, as far as we know, this is the first
time to find a paradigm in experimentally available
material which visually maps the LC in real space to the
band topology in momentum space. For example in a
TCI family of Ba\( _3 \)Cd\(_2 \)As\(_4 \) \([38]\), it also can be considered
as a LC: \((001; 1) \otimes (001; \frac{1}{2})\), but it can’t give a image that
directly corresponds to the crystal structure in real space.
This perfect paradigm is a good platform to understand
the underlying physics of TCIs and the relationship be-
tween TIs and TCIs.

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* Those authors contributed equally to this work.
1 Electronic address: cfang@iphy.ac.cn
‡ Electronic address: hmweng@iphy.ac.cn
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FIG. 4: (Color online) The spectra of Wilson loop and SS band structures on surface BZ of (100) (a-c) and (110) (d-f) surfaces, respectively. (b, e) The zoomed in image of the shadowed part in (a) and (d), respectively. It can be seen clearly that there are hourglass-like SSs in (b, c) but trivial SSs with full gap in (e, f).

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SUPPLEMENTARY MATERIAL

A. Single-layer calculations of $\sigma$-LaSbTe

FIG. S1: (Color online) Single-layer calculations for one QL and two distorted QLs of $\sigma$-LaSbTe. The corresponding primitive cell is represented by a blue box in (a) and (e), respectively. Calculated band structure along the high-symmetry lines within GGA without (b,f) and with (c,g) SOC for one QL and two QLS of $\sigma$-LaSbTe, respectively. (d) The 2D BZ for these two single-layer structures and the number in parentheses near high symmetrical momenta are the number of occupied Kramer pair bands with negative parity eigenvalues for one QL of $\sigma$-LaSbTe in order to determine the time-reversal $Z_2$. (h) The calculated time-reversal $Z_2$ in $k_z = 0$ with Wilson-loop method for two QLS of $\sigma$-LaSbTe, where the red dashed line is a reference line.

In this section, we check whether one QL of $\sigma$-LaSbTe is a 2D TI and two QLS of $\sigma$-LaSbTe is trivial insulator. First, we construct corresponding single-layer structure for these two cases as shown in Fig S1(a,e). Then we compute the band structures without and with considering SOC. As we can see, without SOC there are one band inversion and double band inversions happened along $\Gamma - Y$ for one QL and two QLS, respectively. When SOC is considered, these two cases are fully gapped so that time-reversal $Z_2$ can be well defined. Since one QL keeps inversion symmetry, the $Z_2$ can be simply derived by Fu-Kane formula. According to Eq.1, we can get $Z_2 = 1$ for one QL. However, for two QLS, inversion symmetry is broken. Therefore, the Wilson-loop method is employed to calculate the wannier-center flow. It’s obvious that $Z_2$ equals zero because the the number of crossings between the Wilson-loop bands and reference line is even. By calculating $Z_2$ index, we confirm each QL of $\sigma$-LaSbTe is a well-defined 2D TI and stacking two weakly coupled 2D TIs can generated a normal insulator with trivial $Z_2$ index.

B. Layer construction of $\sigma$-LaSbTe

The “layer construction” method has been introduced to mapping symmetry-based indicator and topological invariants [1]. For $\ell$-LaSbTe with SG. P4/mnm, our convention is the same as Ref [1], so we can directly use the eLC of SG.129 as given in Supplementary Table 5 of Ref [1]. However, for $\sigma$-LaSbTe with SG. Pmcn in this work, the convention is different from Ref [1]. Thence we derive the eLC of SG. Pmcn and tabulate it in Table S1. The second eLC $(001; 1_4)$ marked with blue in Table S1 represents the eLC of $\sigma$-LaSbTe.

| (hkl; d) | $Z_{2,2,2,4}$ | weak | $m_{100}^{000}$ | $g_{010}^{010}$ | $g_{001}^{001}$ | $i$ | $2_{100}^{200}$ | $2_{010}^{201}$ | $2_{001}^{200}$ |
|----------|---------------|------|----------------|----------------|----------------|-----|----------------|----------------|----------------|
| 001:0    | 0000          | 0000 | 00             | 1              | 1              | 0   | 0              | 1              | 1              |
| 001:1_4  | 0002          | 0000 | 00             | 1              | 0              | 1   | 1              | 0              | 1              |
| 100:1_4  | 0000          | 0000 | 20             | 0              | 1              | 0   | 1              | 0              | 1              |
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