Preservation of the twin-plane topology against crystalline symmetry breaking

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INTRODUCTION

- Topological crystalline insulators (TCIs) are materials in which crystal symmetry protects the non-trivial topology of the electronic band structure [1]. In SnTe material class the negative bulk band gap leads to Dirac-like metallic surface states which are protected by {110} mirror symmetries.
- We have recently shown that twin planes (TPs), as a planar defect in SnTe with rocksalt structure, can be treated as 2D topological structures belonging to the TCI class which are protected by the (111) mirror symmetry. The value of the topological invariant - the mirror Chern number - depends on the type of twinning and is equal to $C_m = 1$ for an anionic TP and to $C_m = 2$ for cationic one [2].
- The entanglement cut technique is used for the topological characterization of a subsystem, such as TP in the twinning superlattices (TSLs) and slab with a single TP [3,4].

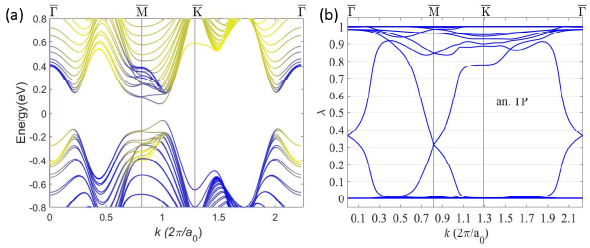
ENTANGLEMENT SPECTRUM: SnTe

correlation matrix:

- $C_A(\boldsymbol{k}) = P_A P_- P_A$
- $C_A(\boldsymbol{k})\tilde{\psi}_n(\boldsymbol{k}) = \lambda_n(\boldsymbol{k})\tilde{\psi}_n(\boldsymbol{k})$

P_A : projection operator onto the subsystem "A"
P_- : projection operator onto the occupied bands
A : can be either TP_1 (T_1), TP_2 (T_2) or bulk (B) region
λ : eigenvalue of the correlation matrix C_A

➢ *Twinning superlattices*



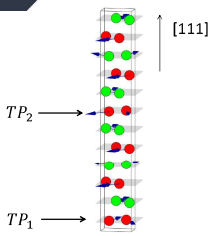
- **Non-trivial** energy gap leads to a gapless entanglement spectrum
- The partition (or cut) is coupled with the environment
- The entanglement mirror Chern number cannot be calculated due to zero gap

Figure 2: (a) The electronic band structure of a 120 monolayer-height supercell of a SnTe an-an TSLs. (b) Gapless entanglement spectra (λ) of a T_1= 41 layer cut, including a single TP in the middle.

BREAKING {110} CRYSTALLINE SYMMETRIES

➢ *SnTe twinning superlattices*

- Perturbation made by a random in-plane atomic shift for a doubled TSL supercell
- The three {110} mirror symmetries are broken
- (111) Mirror symmetry is preserved



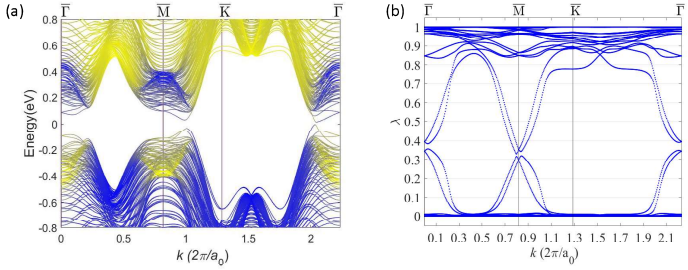
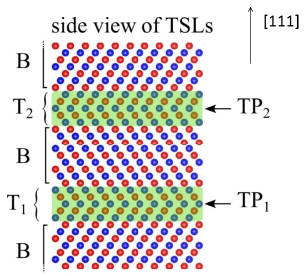


Figure 4: (a) The electronic band structure of a 120 monolayer-height *doubled* supercell of a SnTe an-an TSLs. (b) The entanglement spectra (λ) of a T_1 = 41 layer cut, including a single TP in the middle. The perturbation is added into the system in order to open entanglement gap.

TWINNING SUPERLATTICES



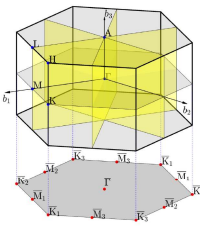
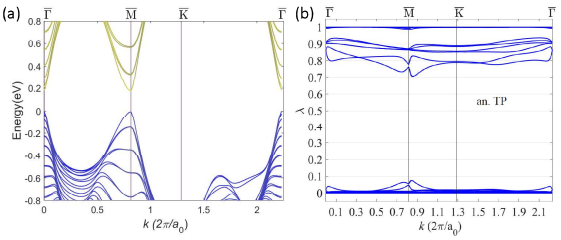


Figure 1: **Left:** Side view of TSLs. **Right:** 3D hexagonal Brillouin zone (BZ) of the TSLs and 2D (111) slab BZ indicated with gray color.

B → bulk-like region, **T_1 → twin plane 1 (TP_1) region,** **T_2 → twin plane 2 (TP_2) region**

ENTANGLEMENT SPECTRUM: PbTe



- **Trivial** energy gap leads to a gapped entanglement spectrum
- The partition (or cut) is disentangled from the environment
- The entanglement mirror Chern number of the partition is zero

Figure 3: (a) The electronic band structure of a 120 monolayer-height supercell of a PbTe an-an TSLs. (b) The entanglement spectra (λ) of a T=41 layer cut, including a single TP in the middle.

ENTANGLEMENT BERRY CURVATURE

➢ *SnTe twinning superlattices*

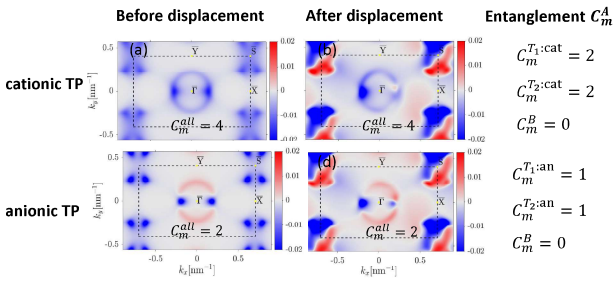


Figure 5: Berry curvature associated with the $-i$ (111) mirror subspace for (a) an-an and (c) cat-cat TSLs without perturbation. Berry curvature associated with the $-i$ mirror subspace for (b) an-an and (d) cat-cat TSLs with perturbation breaking {110} bulk crystalline symmetries. Calculations were performed with a 120 monolayer-height supercell.

➢ *(111) SnTe Slab with a single TP*

- The same approach applied for a (111) SnTe slab with a single TP
- After adding perturbations and breaking crystalline symmetries other than (111) mirror plane, we obtain that:
  1. The bulk-like contributions to the Berry curvatures are zero
  2. The top and bottom surface contributions to the Berry curvatures are zero
  3. The TP region contributions to the Berry curvatures are nonzero, and the entanglement mirror Chern number is $C_m^{TP} = 1$ for the slab built with anionic TP and $C_m^{TP} = 2$ for the slab built with cationic TP.

CONCLUSIONS

- Inverted gap at the L points in bulk BZ is crucial for the nontrivial properties of TPs.
- Preservation of crystalline symmetries of the defect free bulk region is not essential as long as (111) mirror TP symmetry is preserved
- Bulk-like contributions to the Berry curvatures are zero.
- The mirror Chern number is the same as in the case studied before [2], even when all crystalline symmetries other than (111) mirror TP symmetry are broken

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