Topological phase transition in SnTe topological crystalline insulator thin films

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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].
- There are many studies of (001) crystallographic orientation surface, including clean (001) surface, steps and films [3-6]. In case of (001) films the nontrivial topology is manifested by a mirror Chern number for odd number of layers. However, for an even number of layers, the winding number ζ_m becomes nontrivial for a certain range of layers [3].

(111) films with a TP

❖ Structure

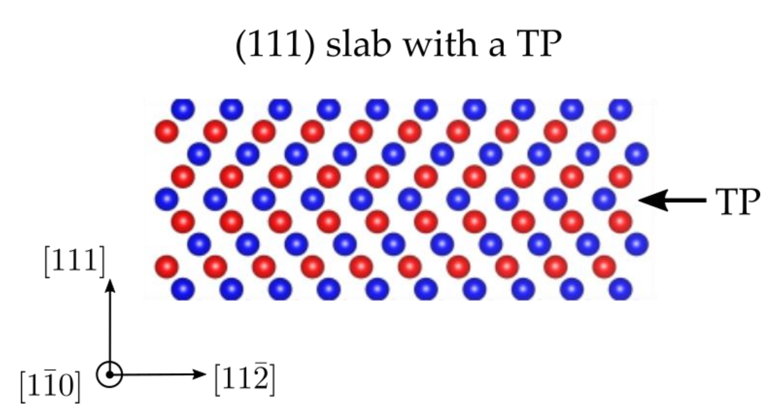


Fig.1. slab structure with a twin plane (TP).

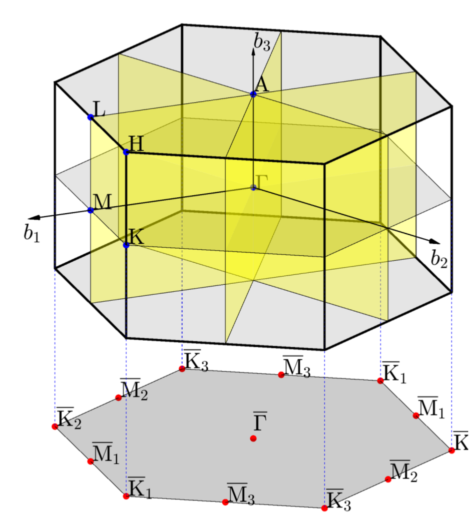


Fig.2. 2D hexagonal Brillouin zone (BZ) of the (111) surface of twinning superlattices (TSLs).

❖ Berry curvatures for twinning superlattices

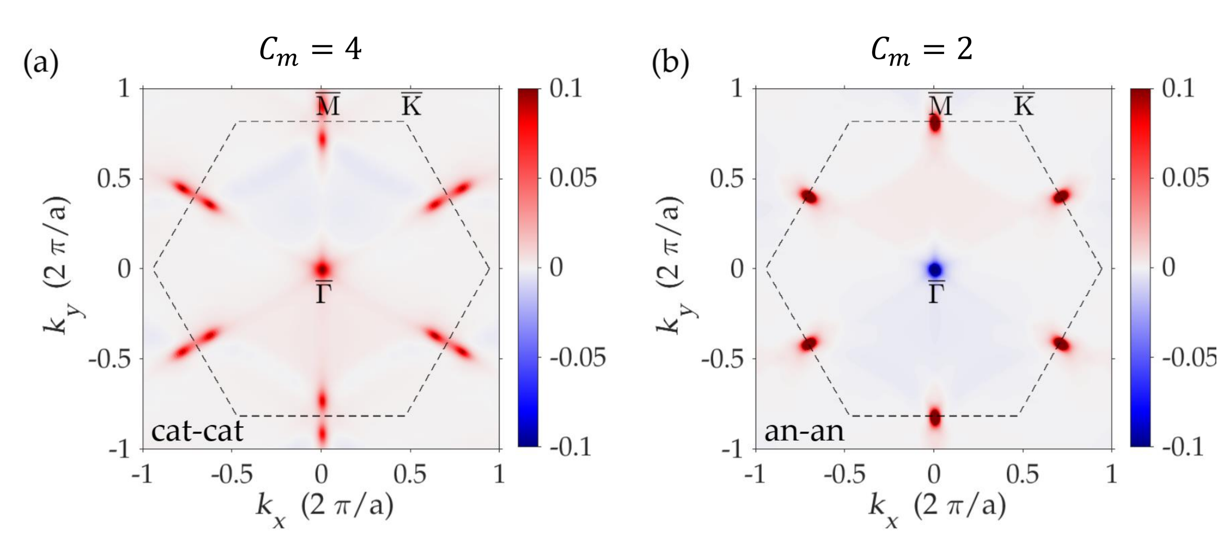
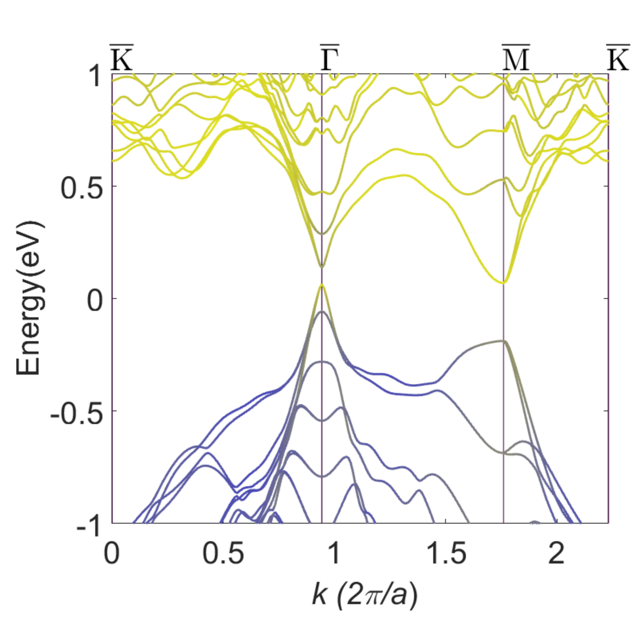


Fig.3. The Berry curvatures related to +i (111) mirror subspace are determined for two types of TSLs: (a) cat-cat TSL and (b) an-an TSL with a height of 32 atomic layers.

❖ Topological phase transitions



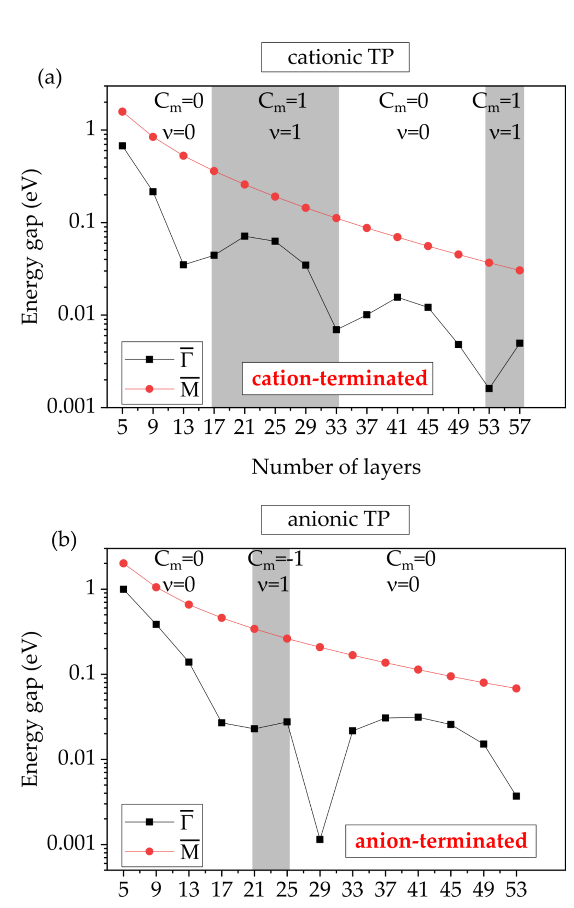


Fig. 4. Left: band structure for 21 atomic layer film with cationic TP and cationic surfaces. Right: Energy gaps in (111)-oriented films with an odd number of monolayers in the presence of TP.

❖ Edge spectral Greens functions

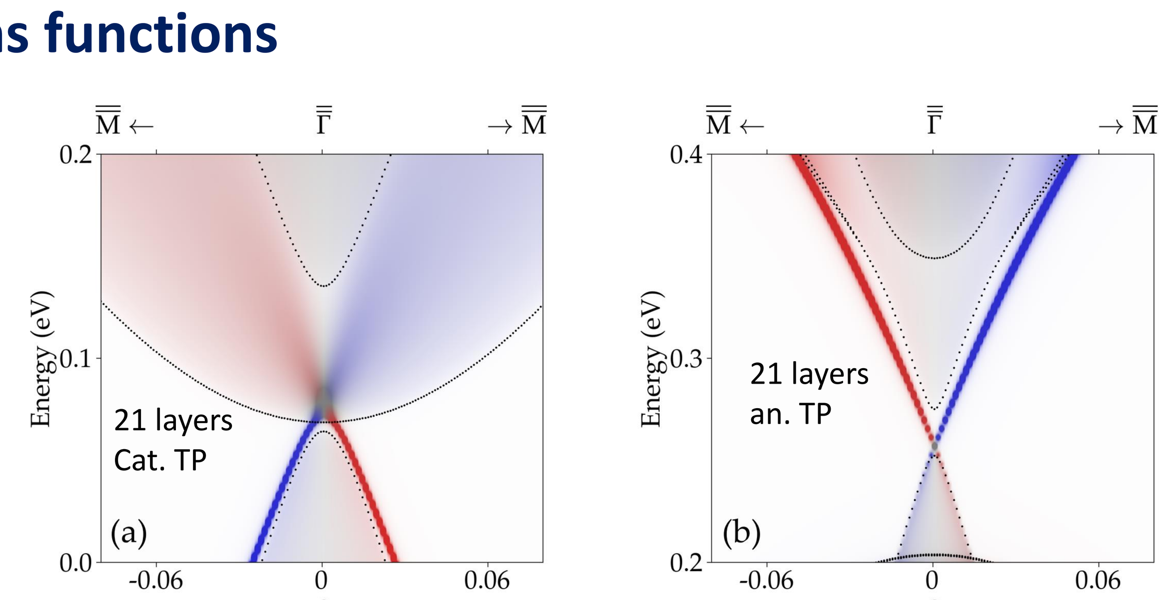
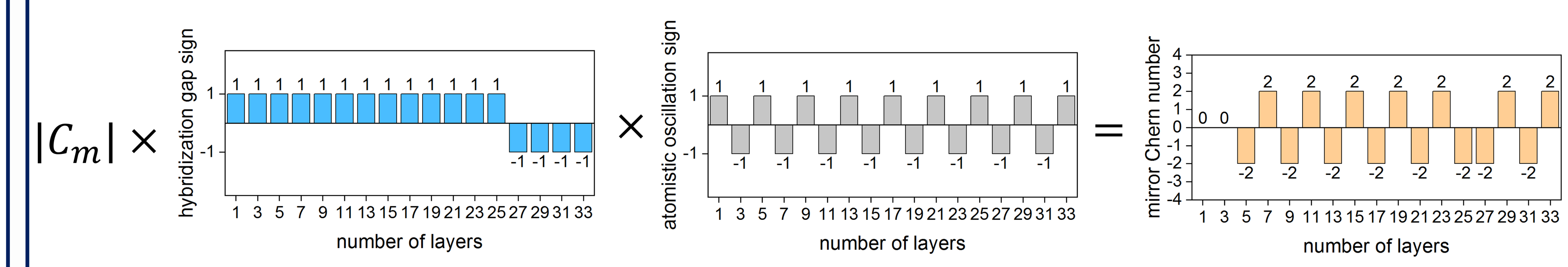


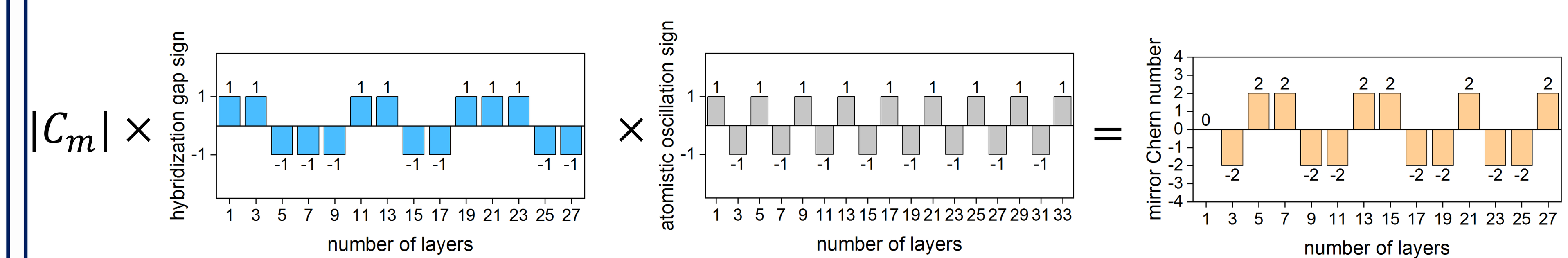
Fig.5. The quantum spin Hall phase at the edge of (111) films with a TP. The red and blue color indicate the spin-down and spin-up polarizations, respectively.

(001) films

❖ (001) Mirror Chern number (C_m)

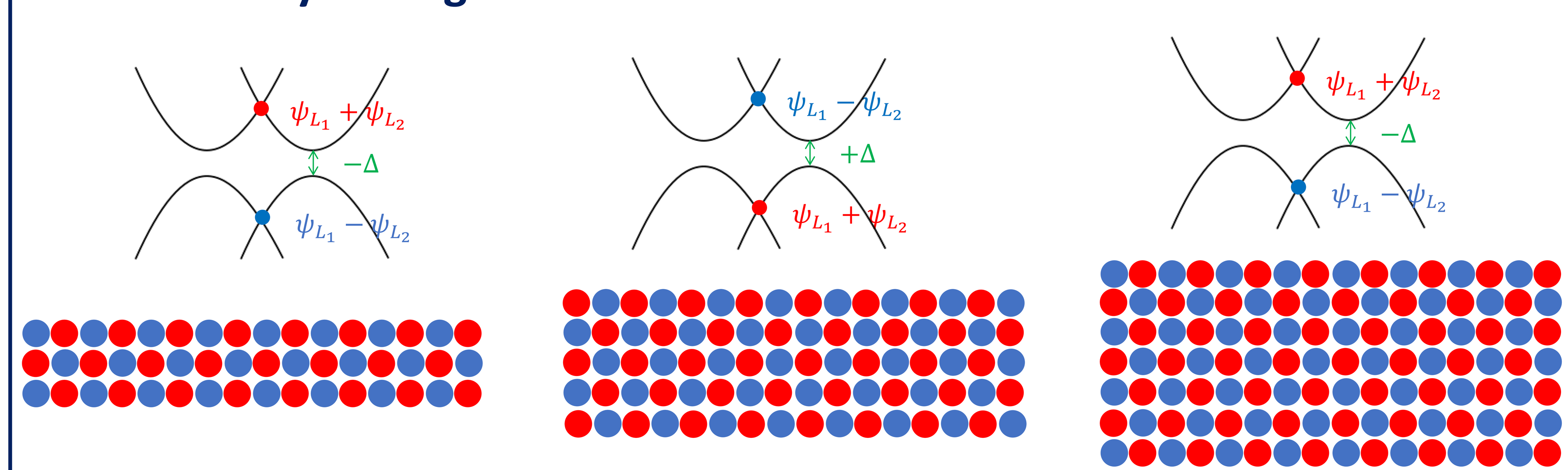


- *Fig.6.* (001) Mirror Chern number in *spd*-orbital SnTe model. Left: is energy gap oscillation due to hybridization between two opposite surfaces (long-period). Middle: The atomistic oscillation of sign of the gap in slabs composed of an odd number of layers due to inter-valley mixing (i,e., fast oscillation). Right: the calculated results of C_m.



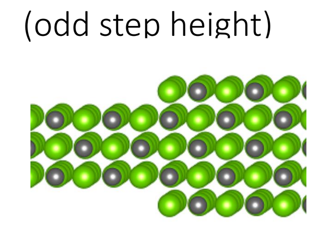
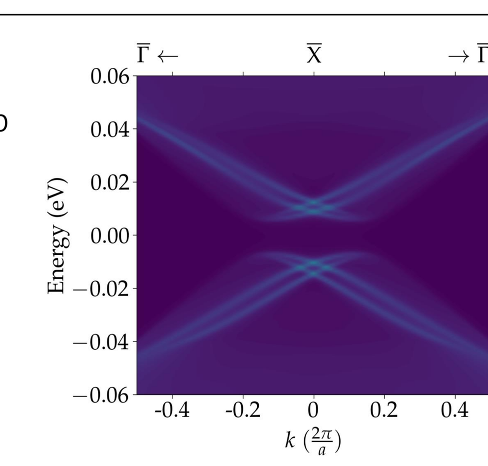
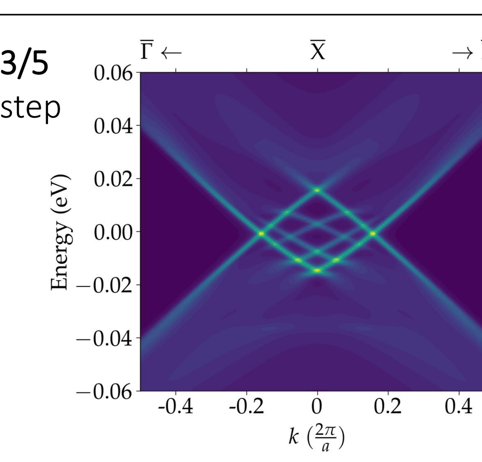
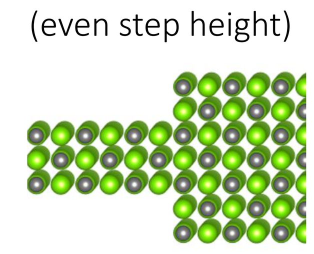
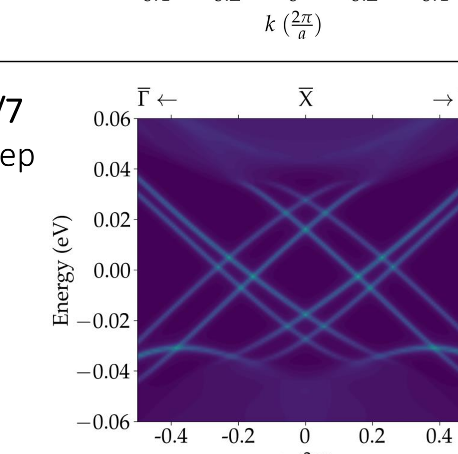
- *Fig.7.* (001) Mirror Chern number in simplified *p*-orbital SnTe model. Left: is energy gap oscillation due to hybridization between two opposite surfaces (long-period). Middle: The atomistic oscillation of sign of the gap in slabs composed of an odd number of layers due to inter-valley mixing (i,e., fast oscillation). Right: the calculated results of C_m.

❖ Inter-valley mixing



❖ Symmetrized step films

The figures below show the calculated edge spectral of (001)-symmetrized-step film.

	$\Delta C_m = 0$	$\Delta C_m \neq 0$
3/5 step (odd step height) 	5/7 step 	3/5 step 
3/7 step (even step height) 	e.g., 19/23 step trivial case – no step-edge modes	3/7 step 

Conclusions

(111) films with a TP

- The TP wavefunctions are mixed with surface states due to small distance of TP and two (111) surfaces.
- The TP topology is fragile and is destroyed by the hybridization of TP wavefunctions with surface states.
- (111) films with cationic or anionic TP exhibit quantum spin Hall phase similar to the pattern observed in (111) films without TP.
- In the limit of sufficiently large (111)-oriented slabs, the hybridizations of two (111) surface wavefunctions become much lower. However, the slabs exhibit gapless surface states band structures, which make it impossible to calculate Chern number.

(001) films

- The mirror Chern number oscillates between C_m=+2 and $C_m = -2$.
- The oscillation of the sign is made up of two components — a slow one due to hybridization gap, and a fast one, due to valley mixing, which changes the sign of C_m with every two added layers.
- Symmetrized steps in slabs host edge states. They are topologically protected if the thicknesses on both sides of the step correspond to different C_m. However, trivial edge states may emerge at steps of odd height, even when $\Delta C_m = 0$.

References

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Acknowledgments

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