Topological phase transition in SnTe topological crystalline insulator thin films

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The quantum spin Hall (QSH) phase was theoretically predicted in (111)-oriented thin films in a certain range of thicknesses in the SnTe class of topological crystalline insulators (TCIs). The energy gap changes sign and oscillates with increasing the number of layers due to intersurface hybridization. This leads to the emergence of the two-dimensional (2D) topological insulator phase classified by a $\mathbb{Z}_2$ invariant protected by time-reversal symmetry [1,2].

We study topological properties of symmetric (111)-oriented films with a twin plane (TP) in the middle of the structure. The TP forms a (111) mirror symmetry plane and can be either cationic or anionic type. Recently, we have shown that both a cationic and an anionic TP defines a 2D TCI with mirror Chern number $C_m = 2$ and $C_m = 1$, respectively [3]. Using tight binding approximation we calculate mirror Chern number and $\mathbb{Z}_2$ invariant for thin films with TPs for a wide range of thicknesses. We show that TP topology combined with finite-size effects can influence how the topological invariants change with growing film thickness.

In addition, we investigate phase transitions in (001) films by calculating the mirror Chern number and find that it oscillates between $C_m = +2$ and $C_m = -2$ with growing thickness. Using a realistic tight binding model we uncover that the oscillation is made up of two components — a slow one described in Ref. [4], and a fast one, due to valley mixing, which changes the sign of C_m with every two added layers. Following Ref. [5] we consider films with atomic steps located symmetrically on the two surfaces. Such steps constitute boundaries between areas of different film thickness. In agreement with Ref. [5], we find that there appear gapless step-edge modes protected by (001) mirror symmetry, whenever the thicknesses on both sides of the step correspond to different values of C_m.

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