

# Magneto-optical determination of the topological character of $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ topological crystalline insulator

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This present work focuses on the study of the electronic properties under magnetic field and the topological character of lead-tin selenide ( $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ ) topological crystalline insulator (TCI) [1]. This semiconductor material belongs to a novel class of topological materials which generally exhibit Dirac-like dispersion of insulating bulk states with band gap coexisting with gapless conducting surface states at the boundaries, as found in the well-known existing  $\text{Z}_2$  topological insulators (TIs) [2]. This intriguing peculiar aspect protected by time-reversal symmetry results directly from the inversion, caused by the spin-orbit interactions, of the lowest conduction and the highest valence bulk bands having different parities. Therefore, the topological character of condensed materials is fundamentally governed by the bulk band parity and orbital ordering. A semiconductor is said to be “trivial” when its bulk bands are normal (with positive band gap), while it is said to be “nontrivial” or “topological” when its bulk bands are inverted (with negative band gap) compared to conventional semiconductor. To change the band ordering, the material must undergo a topological phase transition from trivial regime to topological regime.

The inversion of the bulk band ordering can also be observed in TCIs such as a narrow gap ( $< 1$  eV) rocksalt IV-VI semiconductor  $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ . For a given temperature, there exists a critical Sn composition  $x_c$  at which the topological phase transition occurs [3]. For  $x < x_c$ ,  $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$  is trivial since it behaves as conventional semiconductor. For  $x > x_c$ , such a material has been shown to display similar insulating bulk states and topological surface states (TSS) as in the case of TIs, but the TSS are protected by the crystalline symmetry of the system. In this work, high-quality (111)-oriented  $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$  ( $0 \leq x \leq 0.3$ ) films epitaxially grown on  $\text{BaF}_2$  substrates by means of molecular beam epitaxy (MBE) were performed at 4.5 K using magneto-optical absorption spectroscopy in the infrared spectral range (4-930 meV) with magnetic field up to 15 T. This principal investigation is an ideal technique used to probe narrow gap semiconductors as it provides quantitative information about the bulk band parameters via the Landau quantization of the electron states [4]. The minima of the transmission spectra correspond to optical transitions between Landau levels. This allows us to extract the band parameters of both the bulk and TSS, i.e. the Dirac velocity and the Dirac mass or the energy gap, of the material using the Dirac fermion model analysis [5,6,7]. Experimental findings from a systematic study demonstrate that a topological phase transition in our TCI  $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$  films takes place in the vicinity of  $x_c \approx 0.16$  [7]. For  $x < 0.16$ , the band gap is positive and the material is in trivial phase, while for  $x > 0.16$  the band gap becomes negative and the material is in topological phase. The latter is confirmed by the observation of the cyclotron resonance of the TSS. The heart of our analysis is the ability to verify whether a material is trivial or topological by comparing the value of a considered bulk Dirac velocity  $v_D$  with the critical Dirac velocity  $v_c$  measured at  $x_c$ . For a Dirac material such as  $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$  that can be described by a Bernevig-Hughes-Zhang (BHZ) Hamiltonian,  $v_D$  and  $v_c$  are related to a topological index  $\eta$  as follows:  $(-1)^\eta = \text{sign}(v_D^2 - v_c^2)$  [7]. We found experimentally that when  $v_D > v_c$ , the material is trivial (positive band gap) and  $\eta = 0$ , while  $v_D < v_c$ , the material is topological (negative band gap) and  $\eta = 1$ . In other words, we are able to determine experimentally the topological index corresponding to the topological character of a Dirac material satisfying a BHZ Hamiltonian via its bulk band properties. This is also confirmed by another work performing magneto-transport experiment on the same  $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$  samples [8]. Our approach can be thus argued to be more or less valid for several other systems that exhibit a topological phase transition and can be described using a BHZ-like Hamiltonian.

## References

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