Probing spatial extent of topological surface states by weak antilocalization experiments

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Weak antilocalization measurements has become a standard tool for studying quantum coherent transport in topological materials. It is often used to extract information about number of conducting channels and dephasing length of topological surface states. We study thin films of prototypical topological crystalline insulator SnTe. To access microscopic characteristic of these states we employ a model developed by Tkachov and Hankiewicz, [Physical Review B 84, 035444]. Using this model the spatial decay of the topological states is obtained from measurements of quantum corrections to the conductivity in perpendicular and parallel configurations of the magnetic field. Within this model we find interaction between two topological boundaries which results in scaling of the spatial decay with the film thickness. We attribute this behavior to bulk reservoir which mediates interactions by scattering events without phase breaking of topological carriers.

Introduction. The existence of topological gapless boundary states is characteristic for topological insulators (TI’s) protected by time reversal symmetry as well as for topological crystalline insulators (TCI’s) governed by specific crystalline symmetry of unit cell.1–7 In three dimensions the boundary states form topological surface states (TSS) with defined spin chirality. This implies their π-Berry’s phase and thus robustness against elastic back-scattering. In high field magnetotransport experiments the Berry’s phase of TSS manifests as an additional phase shift in Shubnikov-de Haas quantum oscillations.8 In the low magnetic field however, the Berry’s phase is responsible for destructive interference of two time reversal quantum-mechanical paths around closed loop. Due to exact quantization of Berry’s phase to π there is no other possibility than this destructive interference which leads to negative quantum correction to resistivity at zero magnetic field. Small magnetic field destroys phase coherence leading to positive magnetoresistance called weak antilocalization (WAL). The observation of this effect is often the first indication that we deal with topologically nontrivial material. To date, all experiments on WAL in TI’s or TCI’s have been focused on measuring angular dependence of the effect to prove its 2D origin. Less attention has been addressed to the field in-plane configuration. A comprehensive theory for intrinsically spin–orbit coupled materials is presented in the Ref. 11. Commonly, the simplified Hikami–Larkin–Nagaoka (HLN) formalism is used for description of the experimental data in magnetic field perpendicular to the layer. It leads to the determination of the dephasing length and total number of conducting channels as a function of the sample thickness or gate bias voltage in many papers devoted to Bismuth based TI’s.12,13 Analogous treatment was used in IV-VI group TCI’s, but the number of experiments is very limited. Already in first report14 the essential role of coupling between top and bottom TSS is underlined and analyzed in thick SnTe samples (thickness ≥ 200 nm) grown on BaF2 (001) substrates. Similar observations reported in Refs. 15 and 16 concerned the SnTe samples grown on BaF2 (111) and CdTe (111) substrates, respectively. In this Rapid Communication we report on growth and weak antilocalization comprehensive study in SnTe as a function of layer thickness, which enabled us to determine the spatial extent of topological surface states. We employ Tkachov and Hankiewicz model17,18 of WAL developed simultaneously for two configurations of the magnetic field with respect to layer: perpendicular and parallel. The formula for perpendicular configuration is essentially identical to simplified formula of HLN11 Parallel field dependence involves except for the dephasing length, the additional parameter describing finite thickness of topological surface states. Such a treatment of effective thickness was already considered in early works on interference corrections to conductivity of 2DEG systems,19,20 but now has found implementation in making complete description of weak antilocalization of TSS. Consequently, the experimental data on weak antilocalization collected in two aforementioned magnetic field configurations provide the information about the effective thickness of TSS.

FIG. 1. (a) RHEED patterns recorded during growth of the 100 nm thick SnTe layer. (b) 004 reflection measured as a function of 2θ/ω (blue), thickness oscillations simulation (red).
Experimental. The SnTe thin layers were grown by molecular beam epitaxy on (001) oriented CdTe(4 μm)//GaAs substrates. All the films were grown at 350°C. Finally the SnTe layers were capped with 100 nm thick CdTe barrier. CdTe cap layer was deposited at 290°C. Carrier density is estimated from Hall measurement at the room temperature and equals p = 2 ± 0.5 × 10^{20} \text{cm}^{-3} for all investigated samples. The structural quality of the samples was controlled in-situ by reflection high energy electron diffraction (RHEED) and ex-situ by High Resolution X-ray Diffraction method (HRXRD) (Figs. 1(a) and 1(b) respectively). Both the substrate and the buffer were examined in detail to determine the possible effect on the growth of the SnTe layer. The tetragonal deformation of the lattice unit was found in the CdTe buffer layer. Biaxial compression along interface GaAs-CdTe causes deformations of roughly 2.5 × 10^{-4} (e_{XX} = e_{YY} = e_{CdTe}) = [a - a_{\text{Relax}}]/a_{\text{Relax}}, a – in-plane lattice parameter, a_{\text{Relax}} - lattice parameter of not deformed CdTe unit). In the SnTe layer, tensile deformation along the CdTe interface was found. This is caused by SnTe-CdTe lattice parameter mismatch (a_{SnTe} = 6.32 Å, a_{CdTe} = 6.48 Å) or by linear thermal expansion coefficient α differences (for the SnTe α is over 3 times larger compared to CdTe). The deformation of SnTe elemental cell along interface is about 0.1%. Quality of CdTe/SnTe interface, is revealed in thickness oscillations, (see Fig. 1(b), blue curve) recorded for reflection 004 as a function of 2θ/ω. The simulation curve (marked red on Fig 1(b)) is calculated to estimate thickness oscillations characteristic of a thin (in this case 98 nm) layer.

The samples for transport measurements of SnTe layer thickness d = 10, 20, 40 and 100 nm were cleaved in the rectangular shape of width W = 1.5 mm×2 mm and length 8 mm×10 mm. The Au/Ti metallic contacts were e-beam evaporated in a standard six probe Hall-bar type configuration.

Figure 2 (a) shows raw data of longitudinal resistance in low field range and the inset presents the whole available field range of 9 Tesla collected at 1.5 K. The positive low field magnetoresistance is superimposed onto quadratic background magnetoresistance of bulk carriers. The small positive magnetoresistance we assign to topological surface states. The conductivity of 2D TSS in the whole manuscript is assumed to be \( \sigma_{xx}^{\text{TSS}} = L/W(1/R_{xx}^{\text{tot}}) \), where L is the distance between voltage probes. It is justified as long as low magnetic field region is considered, where \( \sigma_{xy} \ll \sigma_{xx} \) holds and \( \sigma_{xx}^{\text{bulk}}(B) \) is nearly constant.

The weak antilocalization phenomenon, in principle, could also be due to bulk states in systems without inversion center where Dresselhaus spin-orbit interaction is present. Also, in uncapped samples the inversion layer on the surface might be formed inducing structure inversion asymmetry (triangular type quantum well) with Bychkov-Rashba spin-orbit interaction. Both scenarios appear unlikely in the studied system. First, SnTe is of rocksalt fcc structure having inversion center at each atom position. Second, our SnTe films are surrounded by CdTe barriers on both sides, which prevents them from adsorption of foreign adatoms on the surface and consequently from the formation of inversion/accumulation layer.

The methodology of studying localization effects of the topological surface states is similar to other two-dimensional systems. In particular, the ideal 2DEG is sensitive only to perpendicular component of the magnetic field. Thus, all the magnetoconductivity traces should merge when plotted as a function of \( B \cos(\theta) \). The real observation is presented in Fig. 2(b), where region of coincidence of the data collected at different tilt angles is limited to very low magnetic fields. One
FIG. 3. Panels (a)-(d) depict magnetoconductance for various sample thicknesses. Green points and lines present measurements for field parallel to the sample surface. Blue points and lines correspond to perpendicular field configuration.

of the possible cause was identified with finite width of 2DEG, which allows nonzero magnetic flux penetrating the 2DEG in the in-plane configuration. An additional ingredient was considered by Sacksteder et al. who analyse the contribution of side walls which also host TSSs. Consequently, the tilted field dependence of magneto-conductivities should not coincide as a function of perpendicular field component.

The aforementioned papers use elastic mean free path \( L_{\perp} \) of the topological surface states in the description of WAL phenomenon. The conductivity of our samples has always a large contribution from bulk states, therefore it is difficult to extract mean free path of TSS. To overcome this issue, we restrict data analysis to smallest number of fitting parameters. This is given by the model proposed by Tkachov and Hankiewicz of half-infinite slab with two-dimensional TSS characterized by their decay length \( \lambda \) into bulk. Additionally, the model introduces only two more parameters – phase coherence length \( L_\varphi \) and \( |N\alpha|_\perp \) - prefactor proportional to the number of independent coherent channels contributing to the conductivity. For completeness, we specify equations (1) and (2) as given in Ref. 15.

\[
\Delta \sigma_\perp (B) = N\alpha \frac{e^2}{\pi h} \left[ \psi \left( \frac{1}{2} + \frac{B_\perp}{B} \right) - \ln \frac{B_\perp}{B} \right], \quad B_\perp = \frac{\hbar}{4 |e| L_\varphi^2}.
\]

\[
\Delta \sigma_\parallel (B) = N\alpha \frac{e^2}{\pi h} \ln \left( 1 + \frac{B_\perp^2}{B_\parallel^2} \right), \quad B_\parallel = \frac{\hbar}{\sqrt{2} |e| \lambda L_\varphi}.
\]

In both equations (1) and (2) the parameter \( \alpha = -1/2 \) denotes the symplectic universality class to which TSS belong. It is multiplied by \( N \) – the number of independent channels contributing to total conductivity. The phase coherence length \( L_\varphi \) is obtained directly from \( B_\perp \) parameter. The parameter \( \lambda \) introduced in Eq. (2) is interpreted as decay length of the wave function of topological surface states. The explicit formula we quote below:

\[
\lambda = \sqrt{\frac{2\hbar B_\perp}{|e| B_\parallel^2}}.
\]

Our fitting protocol relied on starting with very low magnetic field region and consecutively extending the fitted data region, simultaneously observing the values of parameters \( (N\alpha \text{ and } B_\perp \text{ or } B_\parallel) \). When parameters did not change much, the region of fit was further extended. The resulting theoretical lines are depicted in Fig. 2(c) and Fig. 3. We attribute the fit deviation at higher fields to increased fitting parameters. This is given by the model proposed by Tkachov and Hankiewicz of half-infinite slab with two-dimensional TSS characterized by their decay length \( \lambda \) into bulk. Additionally, the model introduces only two more parameters – phase coherence length \( L_\varphi \) and \( |N\alpha|_\perp \) - prefactor proportional to the number of independent coherent channels contributing to the conductivity. For completeness, we specify equations (1) and (2) as given in Ref. 15.

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\Delta \sigma_\parallel (B) = N\alpha \frac{e^2}{\pi h} \ln \left( 1 + \frac{B_\perp^2}{B_\parallel^2} \right), \quad B_\parallel = \frac{\hbar}{\sqrt{2} |e| \lambda L_\varphi}.
\]

In Fig. 4 we show the results of such theoretical fits for perpendicular field configuration. In the situation studied, i.e. (001) oriented SnTe films, we expected four conducting channels coming from four Dirac cones for both surfaces. Thus in the case of non-interacting channels the \( |N\alpha|_\perp = 4 \times 2 \times 1/2 = 4 \). Instead we obtain with a good accuracy \( |N\alpha|_\perp = 1/2 \) for all samples studied in a broad range of temperatures (see Fig. 4(a)).
FIG. 5. (a) Dephasing length extracted from the Eq. 1 fit in the perpendicular configuration at 4.2 K for various thicknesses. (b) λ as calculated from Eq. 2 for as a function of film thickness. (c) Cartoon depicting modulus squared of the TSS wavefunction decaying exponentially into the bulk reservoir.

We interpret this finding along scenario already pointed by Fukuyama \cite{22} in early studies of Si-MOS magnetococonductivity. Namely, in the case of scattering between $n_v$ valleys the coefficient $n_v\alpha$ becomes renormalized to $n_v\alpha/n_v$ leaving in effect prefactor as for a single conducting channel $\alpha = -1/2$. The same argument applies to the situation of scattering between top and bottom TSS with the help of bulk states reservoir \cite{23,24}

Fig. 4(b) shows the temperature dependence of the dephasing length fitted with exponential formula $L_\varphi \propto T^{-p/2}$. The exponent $p \approx 2$ within experimental accuracy, which is characteristic for electron–phonon interactions dominating at this temperature range \cite{25,26}. The existence of fully degenerate conduction channels is also confirmed in thickness dependence of dephasing length depicted in Fig. 5(a). In case of non-interacting top and bottom TSS the dephasing length should be independent of thickness. Now in opposite case, the quantum interference path started at top TSS continues with the help of bulk reservoir states to the back TSS and returns to the starting point on top surface by scattering events within the bulk. This implies rising phase coherence length with sample thickness.

The main advantage of the Tkachov and Hankiewicz theory \cite{17,18} relies on supplying weak antilocalization formula (see Eq. 2) for in-plane configuration. It enabled us to determine directly the decay length of TSS. The result of such an evaluation is summarized in Fig 5(b). Surprisingly we find $\lambda$ varying with the layer thickness. Without intersurface coupling one could expect $\lambda$ to be thickness independent. However, with our experimental accuracy we determine its value to be about 40% of actual film thickness. The schematic picture is presented in Fig. 5(c), where square of the wave function of the TSS of both, top and bottom surfaces decay exponentially towards the bulk reservoir interior. We emphasize that TSS’s wavefunctions do not hybridize with each other. The high values of $\lambda$ are consequence of interaction of TSS with the bulk reservoir. The presented phenomenological description is in accord with recent tight binding calculations which describe wave function envelope of TSS on the border between trivial and inverted-band regions \cite{20,21}.

Conclusions. In summary, we report on growth of high quality SnTe (001) topological crystalline insulator layers on top of CdTe(4 µm)/GaAs (001) substrate. The SnTe films were capped with 100 nm thick CdTe layer to ensure the same trivial band – TCI interface on both sides of the sample. The weak antilocalization measurements revealed the existence of the two-dimensional topological states. We performed the analysis of low field magnetococonductivity in both perpendicular and in-plane magnetic field orientation. Within Tkachov and Hankiewicz model we found decoherence length depending on the SnTe layer thickness and only one coherent channel taking part in conduction instead of eight expected. Our interpretation relies on assumption of intervalley scattering within one topological surface and intersurface scattering mediated by bulk reservoir. Both lead to eight-fold degeneracy which renormalizes the coefficient in WAL expression to one characteristic for single channel only. In this communication we extended the WAL data analysis by additional parameter describing the spatial extent of the wave function of TSS. We found it depending linearly on the SnTe layer thickness and only one coherent channel taking part in conduction instead of eight expected. Our interpretation relies on assumption of intervalley scattering within one topological surface and intersurface scattering mediated by bulk reservoir. Both lead to eight-fold degeneracy which renormalizes the coefficient in WAL expression to one characteristic for single channel only.

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