Observation of a macroscopic topological insulator phase in thin films of coupled Bi_2Se_3 nanocrystals

Diptiman Sen

Indian Institute of Science, Bengaluru

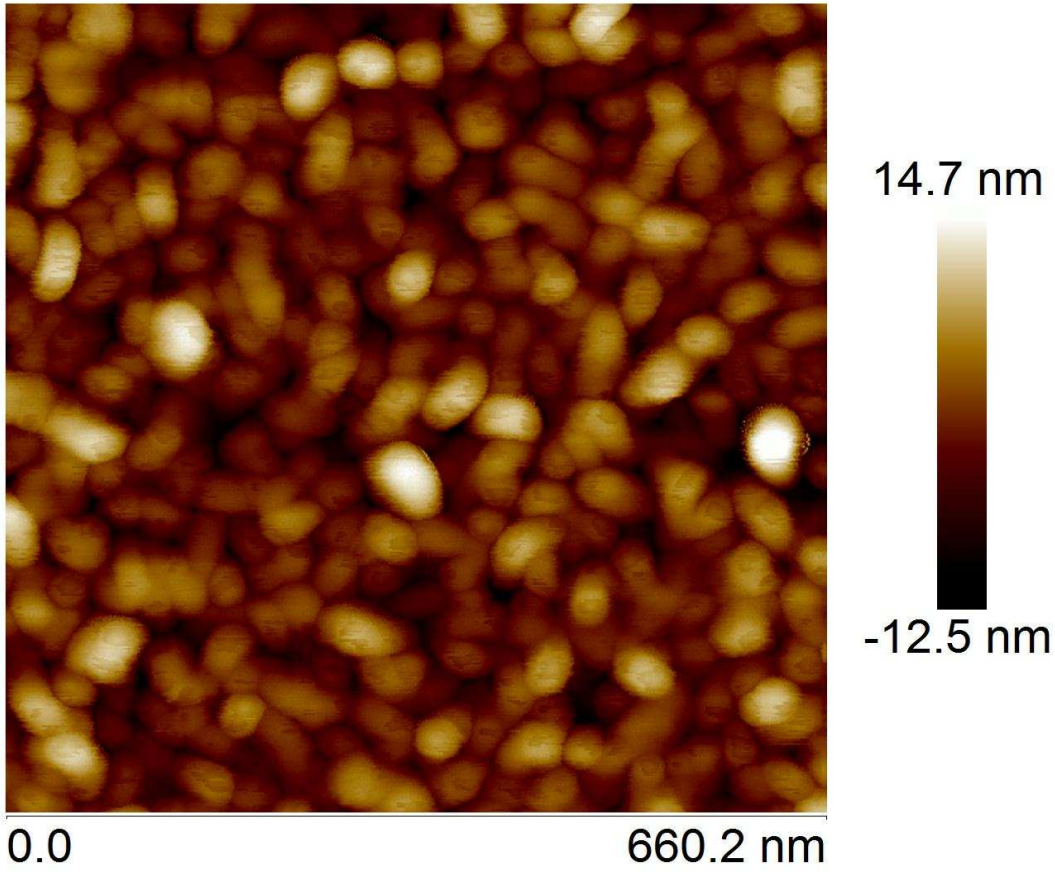
Email: diptiman@cts.iisc.ernet.in

A. Banerjee, O. Deb, K. Majhi, R. Ganesan, D. Sen and P. S. Anil Kumar, arXiv:1604.03767

Outline

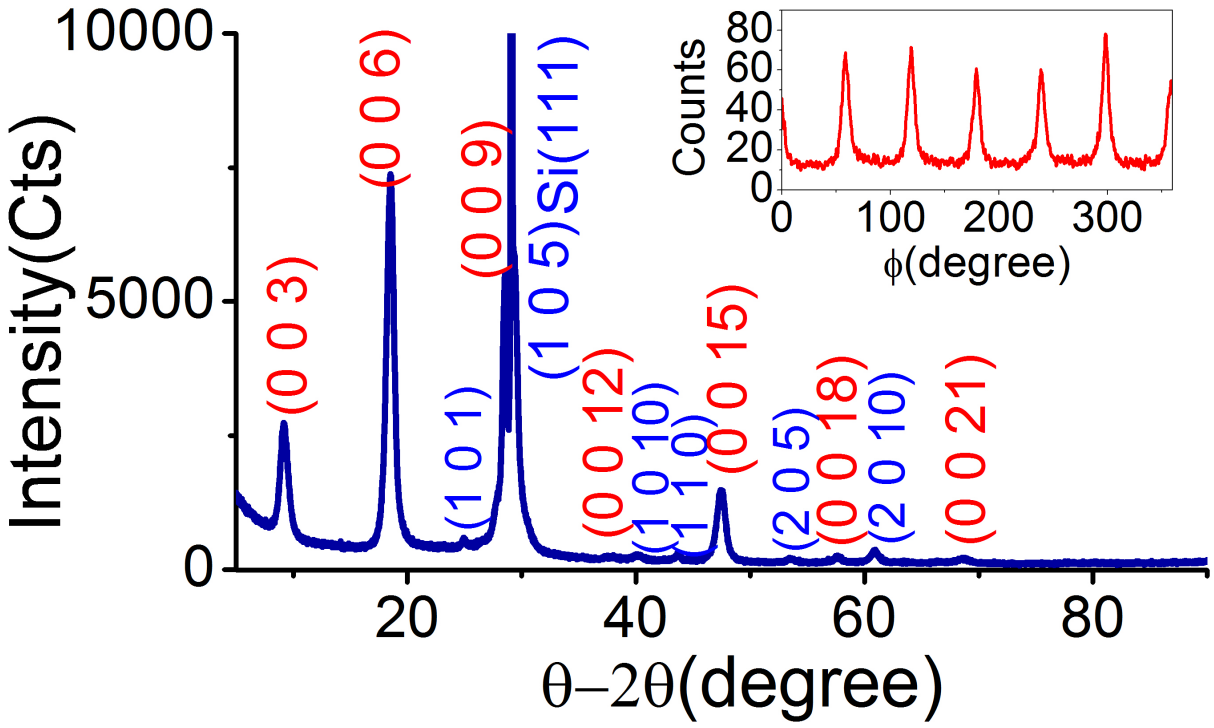
- Thin films of Bi_2Se_3 nanocrystals
- Magnetoconductance data
- Surface penetration depth
- Spin-orbit coupling and Berry phase
- Model of a granular topological insulator

System of Bi_2Se_3 nanocrystals



AFM image showing surface topography of a thin film of Bi_2Se_3 nanocrystals

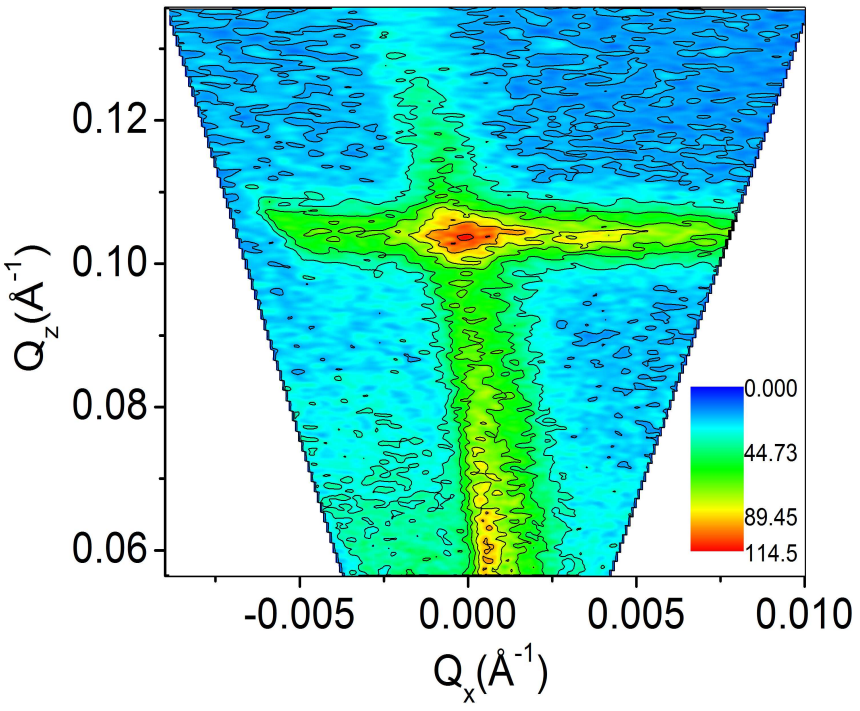
XRD scan showing preferential orientation



Peaks at (003n) imply a preferential orientation along the *c*-axis

Inset: Azimuthal scan of (105) planes of Bi_2Se_3 shows a six-fold symmetry

Reciprocal space map shows granularity



Reciprocal space map of (003) peak shows a large degree of granularity

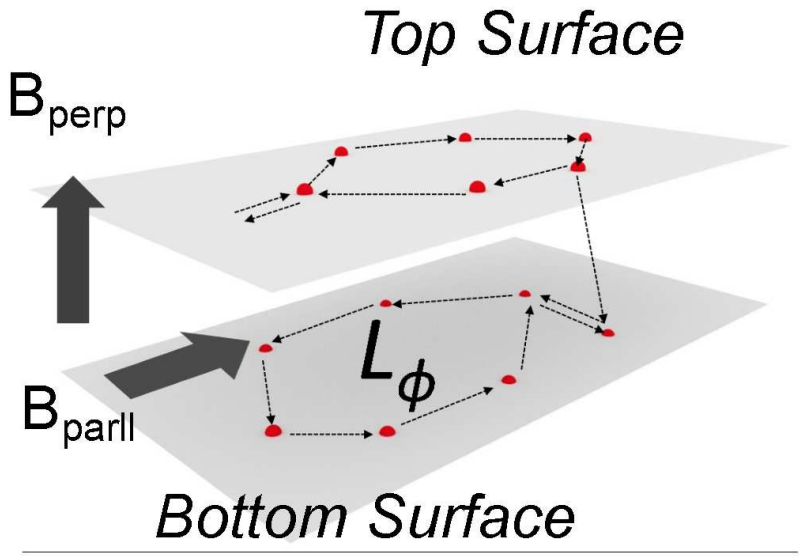
The nanocrystals have a *c*-axis thickness of about 2-3 nm and an in-plane size of about 10 nm

Weak antilocalization

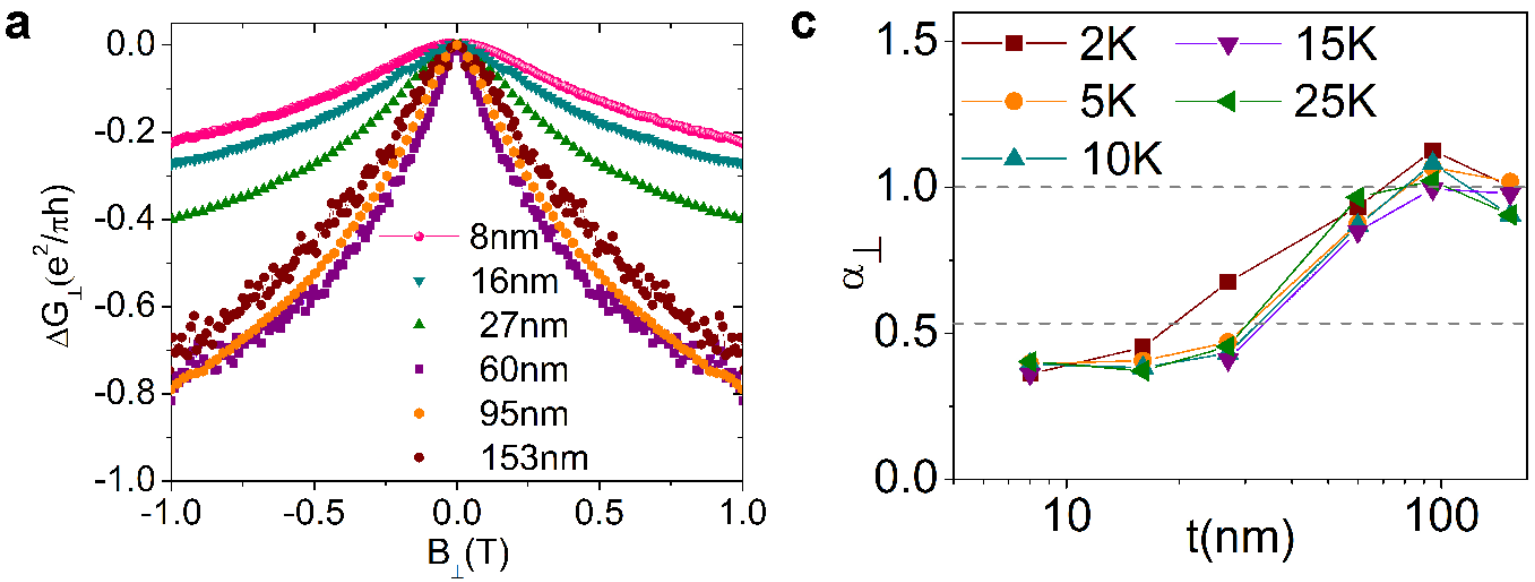
For electrons governed by the massless Dirac equation, the magnetoconductance is negative for small magnetic fields

At zero field, the contributions of a closed path starting and ending at a given point and its time reversed path cancel as they have opposite signs; the Berry phase Φ_B is equal to π. Hence the probability of returning to the same point is reduced and the conductance increases

For a small field, Φ_B moves away from π as the Aharonov-Bohm phases for the two paths are opposite in sign. The probability of returning to the same point increases, and the conductance decreases



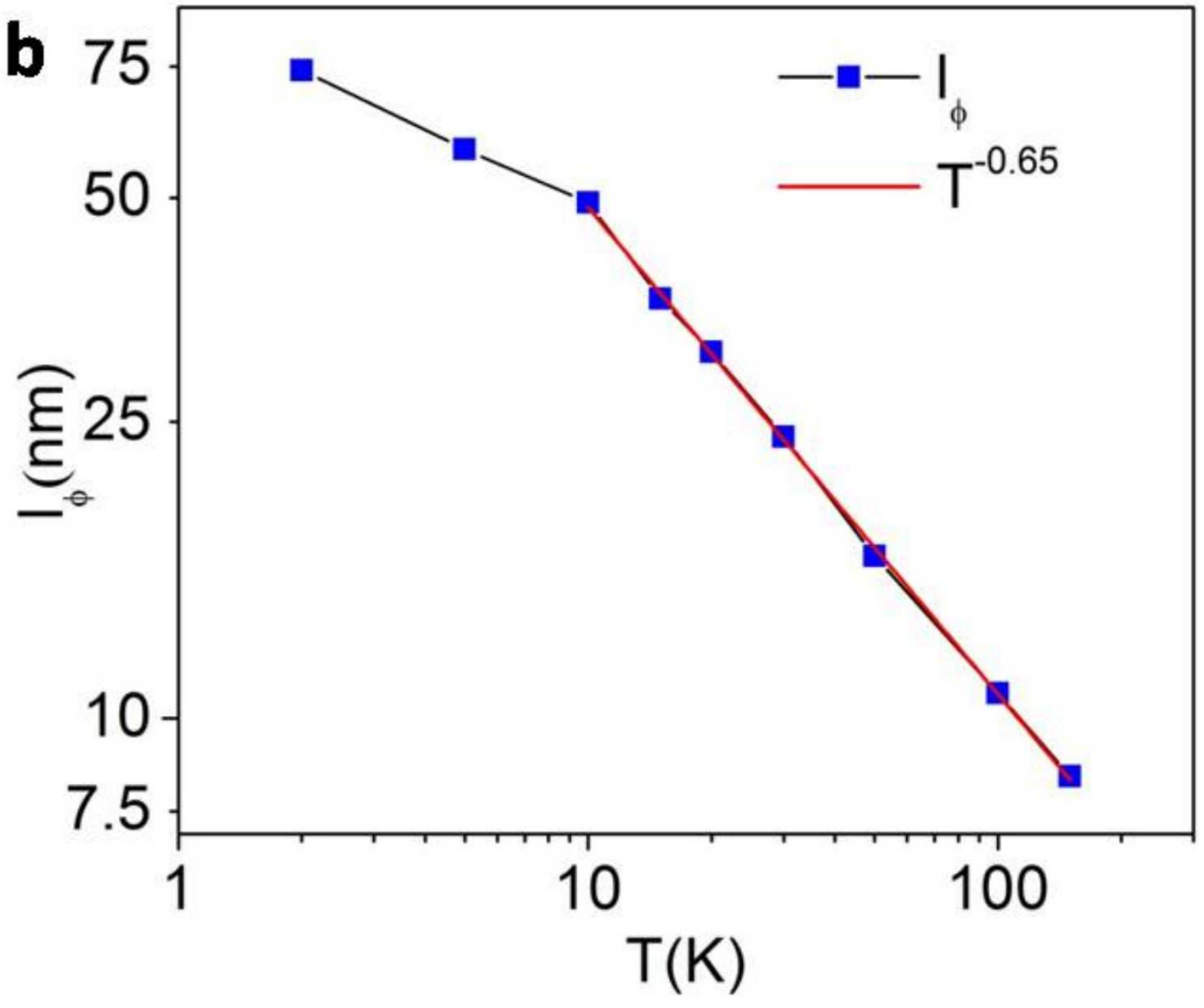
Magnetoconductance for perpendicular field



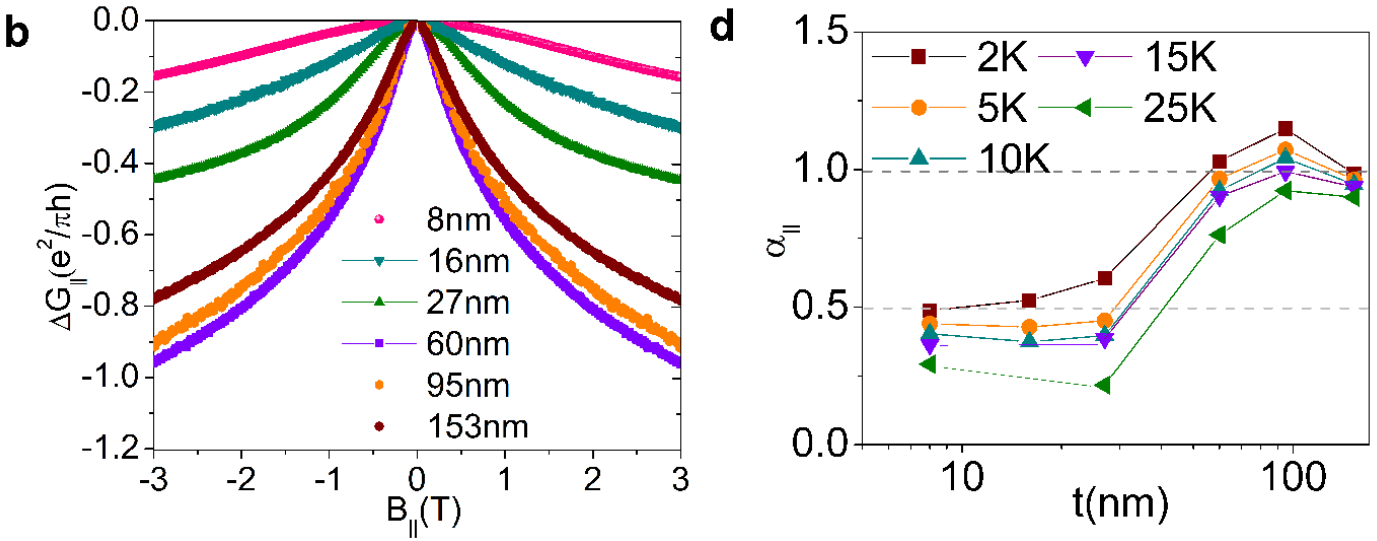
We find $\alpha_\perp$ and l_ϕ (phase coherence length) by fitting the magnetoconductance to the Hikami-Larkin-Nagaoka (HLN) formula

$$\Delta\sigma_\perp(B_\perp) = \alpha_\perp \frac{e^2}{2\pi^2\hbar}\left[\psi\left(\frac{1}{2}+\frac{\hbar}{4el_\phi^2 B_\perp}\right) - \ln\left(\frac{\hbar}{4el_\phi^2 B_\perp}\right)\right]$$

Phase coherence length



Magnetoconductance for parallel field

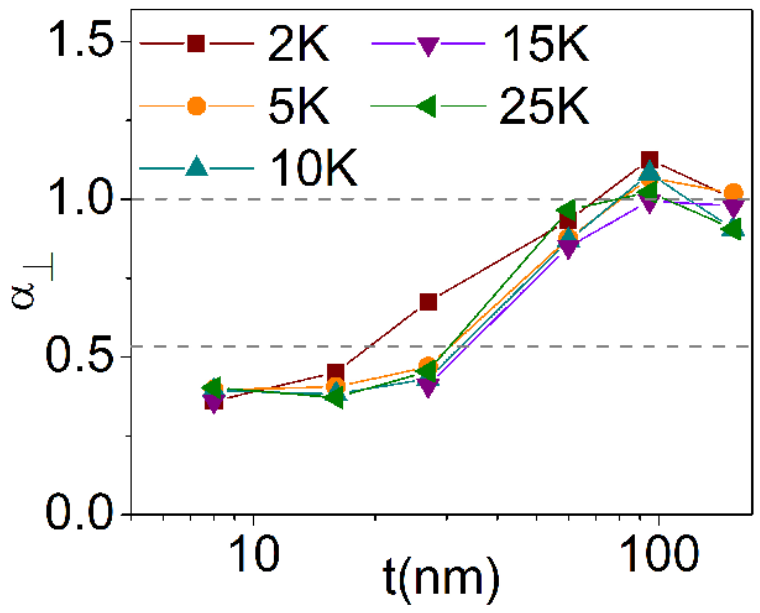


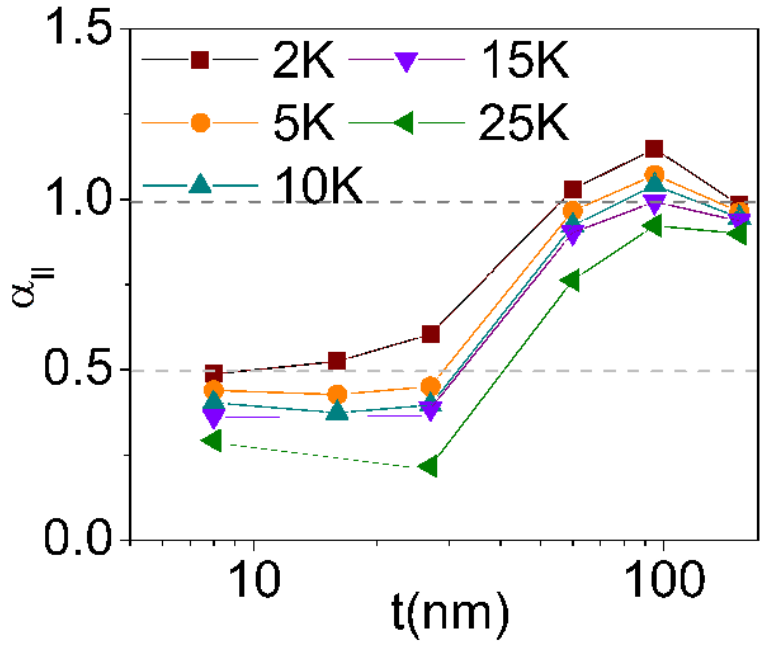
We find $\alpha_{\parallel}$ and λ (penetration depth of surface states) by fitting this magnetoconductance to another HLN formula

$$\Delta\sigma_{\parallel}(B_{\parallel}) = \alpha_{\parallel}\frac{e^2}{2\pi^2\hbar}\ln\left(1 + B_{\parallel}^2/B_{\phi}^2\right)$$

where $B_{\phi} = \hbar/(e\lambda l_{\phi})$, and we use the value of l_{ϕ} obtained from the perpendicular field magnetoconductance data

Comparison between α parameters





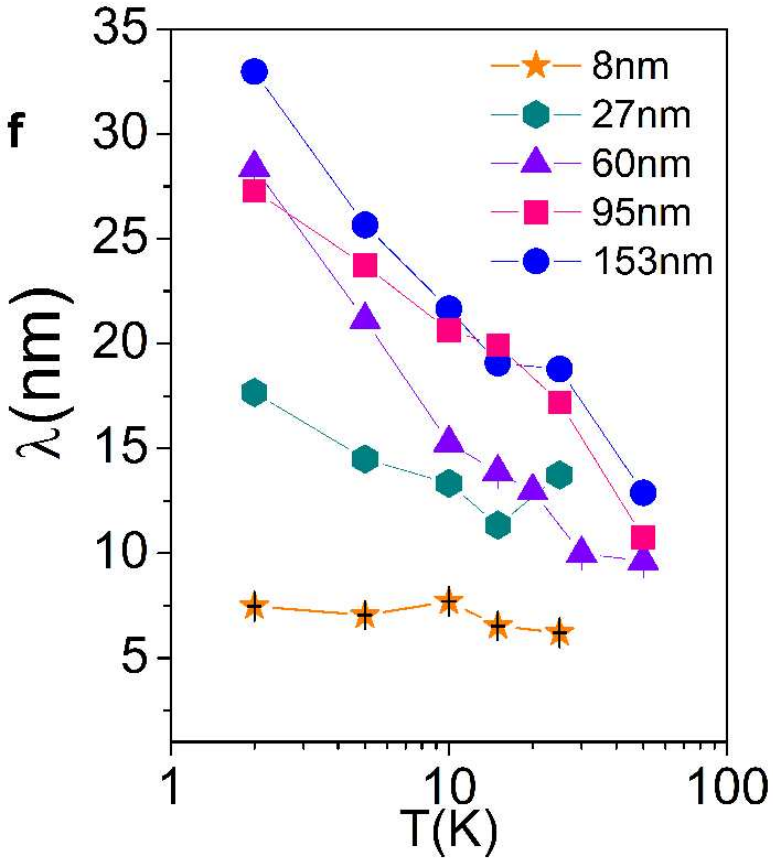
The parameters $\alpha_\perp$ and $\alpha_{||}$ agree well for different film thicknesses

For thick films, they have the value ~ 1 which implies the presence of two decoupled surface states

For thin films, their value ~ 0.5 suggests that the surface states have hybridized

Garate and Glazman, Phys. Rev. B 86, 035422 (2012)

Surface state penetration depth



λ decreases with increasing temperature. Note that the values are much larger than in a single crystal of Bi_2Se_3 where $\lambda \sim 0.8$ nm

Effective spin-orbit coupling and Berry phase

The electrons on the surfaces of a topological insulator (TI) are described by a Dirac equation, with the dispersion $E = v_F|k|$

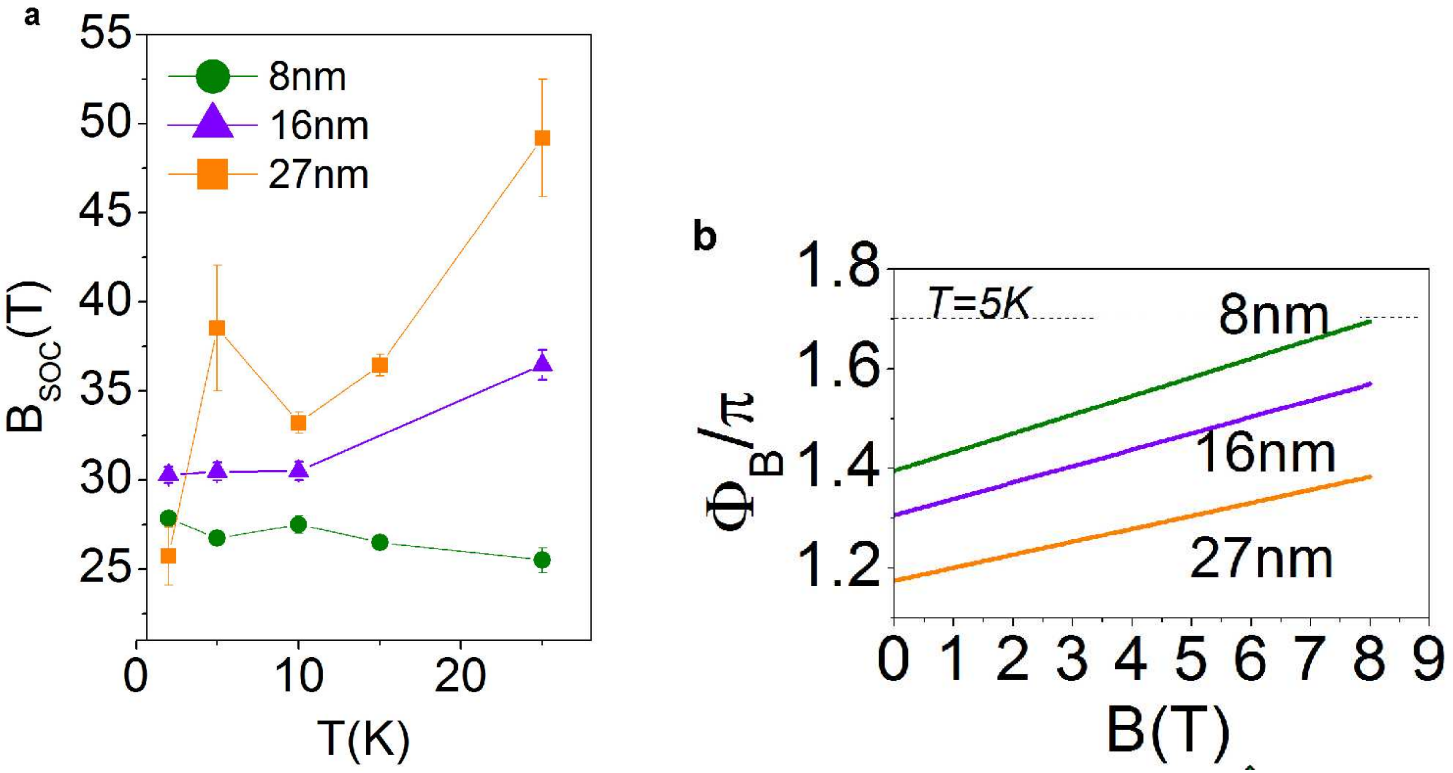
For such an electron, the Berry phase picked up on going around an equal-energy circle in momentum space is π, provided that no magnetic field is present

If there is a magnetic field with a Zeeman coupling to the electron spin, the Berry phase changes from π. Phenomenologically, this modifies the HLN formula to

$$\Delta\sigma_\perp(B_\perp) = \alpha_\perp\left[1-2(B_\perp/B_{SOC})^2\right]\frac{e^2}{2\pi^2\hbar} \times\left[\psi\left(\frac{1}{2}+\frac{\hbar}{4el_\phi^2B_\perp}\right)-\ln\left(\frac{\hbar}{4el_\phi^2B_\perp}\right)\right]$$

where $B_{SOC} = v_F k_F$ is the effective spin-orbit coupling

Effective spin-orbit coupling and Berry phase



The effective spin-orbit coupling B_{SOC} increases with increasing temperature and film thickness

The Berry phase Φ_B moves away from π with increasing magnetic field

$Bi_2\,Se_3$

In a single crystal of $Bi_2\,Se_3$, the Hamiltonian near the Γ point is given by

$$H_{TI} = -m\,\tau^z + \hbar v_z\,\tau^y\,k_z - \hbar v_{||}\,\tau^x\,(\sigma^x k_y - \sigma^y k_x)$$

where the τ^a are pseudospin matrices:
$\tau^z = \pm 1$ denote Bi and Se electrons respectively

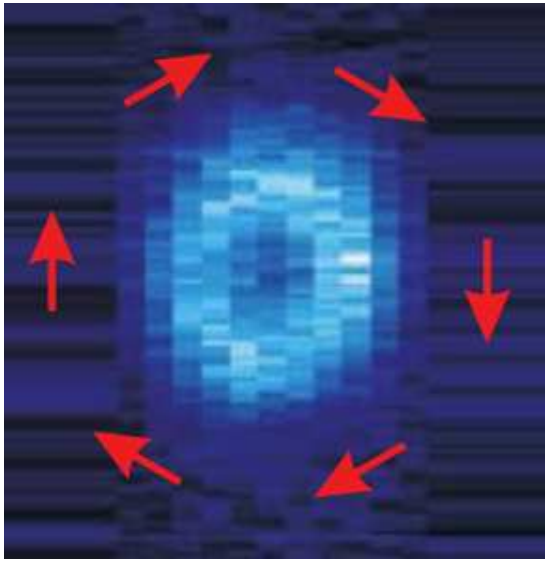
The parameter value are $m = 0.28$ eV, $\hbar v_z = 0.226$ eV nm, $\hbar v_{||} = 0.333$ eV nm

We find both bulk states and surface states. The bulk states are separated from the surface states by a gap equal to 0.28 eV

The surface states decay exponentially as we go into the bulk, with a decay length given by $\hbar v_z/m = 0.81$ nm

$Bi_2 Se_3$

The surface states are described by massless Dirac equations, $H = \hbar v_F (\sigma^x k_y - \sigma^y k_x)$ at the top surface, and $H = -\hbar v_F (\sigma^x k_y - \sigma^y k_x)$ at the bottom surface, where $\hbar v_F = \hbar v_{||} = 0.333$ eV nm. The states show spin-momentum locking; the spin and momentum are mutually perpendicular



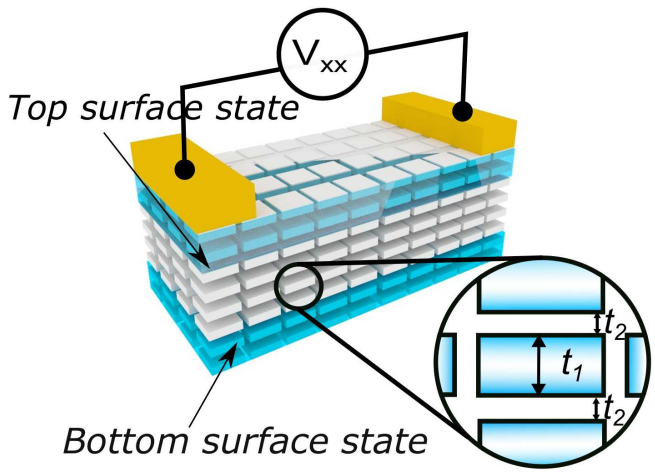
Qi and Zhang, Rev. Mod. Phys. 83, 1057 (2011)

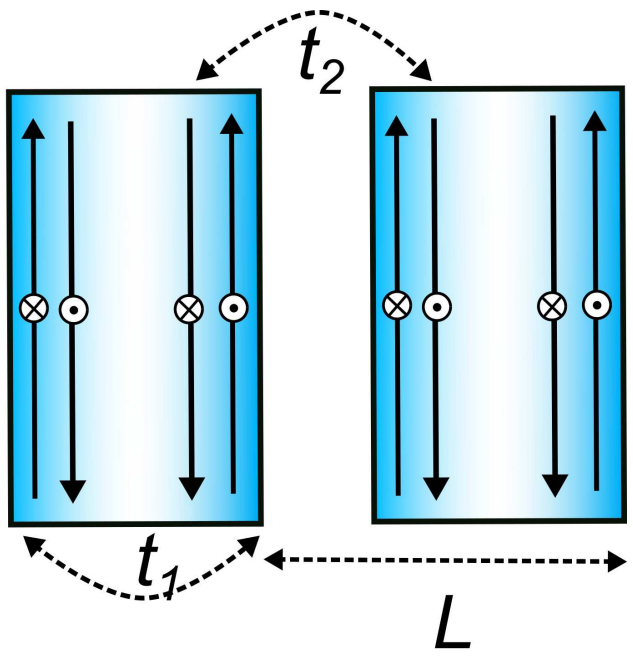
Hasan and Kane, Rev. Mod. Phys. 82, 3045 (2010)

Model of a granular TI

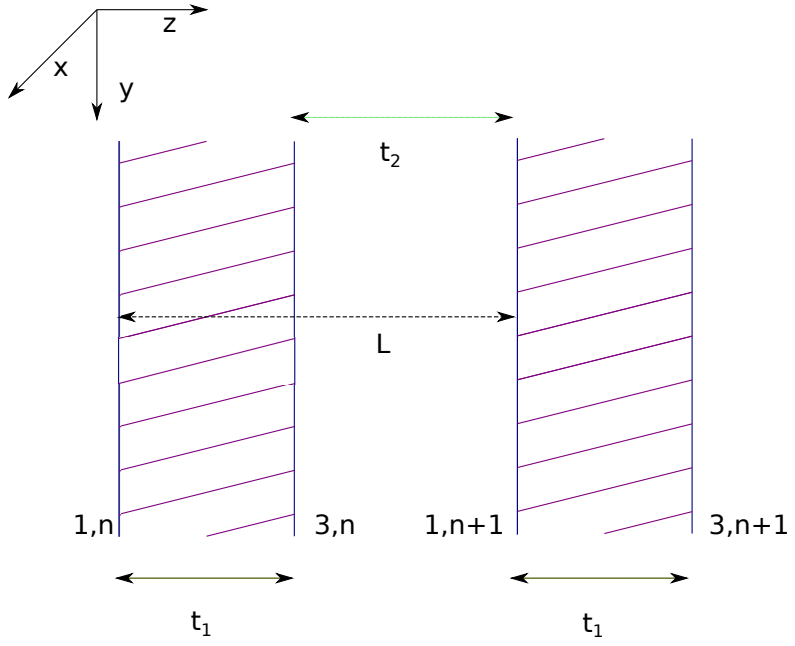
Since the bulk states are separated from the surface states by a gap equal to 0.28 eV in a single crystal of $Bi_2 Se_3$, we will ignore the bulk states of the individual nanocrystals

We introduce couplings t_1 between the top and bottom surfaces of each nanocrystal and t_2 between the surfaces of two neighboring nanocrystals





Surface state couplings t_1 and t_2



Array of grains along the c-axis with a unit cell size L.
Each grain has surfaces 1 and 3 lying in the $x-y$ plane

The surface states are coupled to each other in two ways.
t_2 is due to thermally assisted tunneling through a barrier formed by the charging energies of neighboring grains. Hence t_2 will increase with increasing temperature. But t_1 will not have a significant temperature dependence

Hamiltonian

The Hamiltonian governing all the surface states is

$$H = \sum_n [\psi^\dagger_{1,n} \hbar v_F(\sigma^x k_y - \sigma^y k_x)\psi_{1,n} - \psi^\dagger_{3,n} \hbar v_F(\sigma^x k_y - \sigma^y k_x)\psi_{3,n} + (t_1 \psi^\dagger_{1,n}\psi_{3,n} + t_2 \psi^\dagger_{3,n}\psi_{1,n+1} + H.c.)]$$

If a Zeeman field $\vec{B}$ is applied, we add a term to the Hamiltonian

$$H_b = -\frac{g\mu_B}{2} \sum_n [\psi^\dagger_{1,n}\vec{\sigma}\cdot\vec{B}\psi_{1,n} + \psi^\dagger_{3,n}\vec{\sigma}\cdot\vec{B}\psi_{3,n}]$$

We first look at the energy spectrum in the absence of a Zeeman field

Bulk and surface states

The system as a whole has bulk states with the dispersion

$$E_{\vec{k}\pm} = \pm\sqrt{\hbar^2 v_F^2(k_x^2+k_y^2) + t_1^2 + t_2^2 + 2t_1 t_2\cos(k_z L)}$$

which has a gap equal to $|t_1 - t_2|$

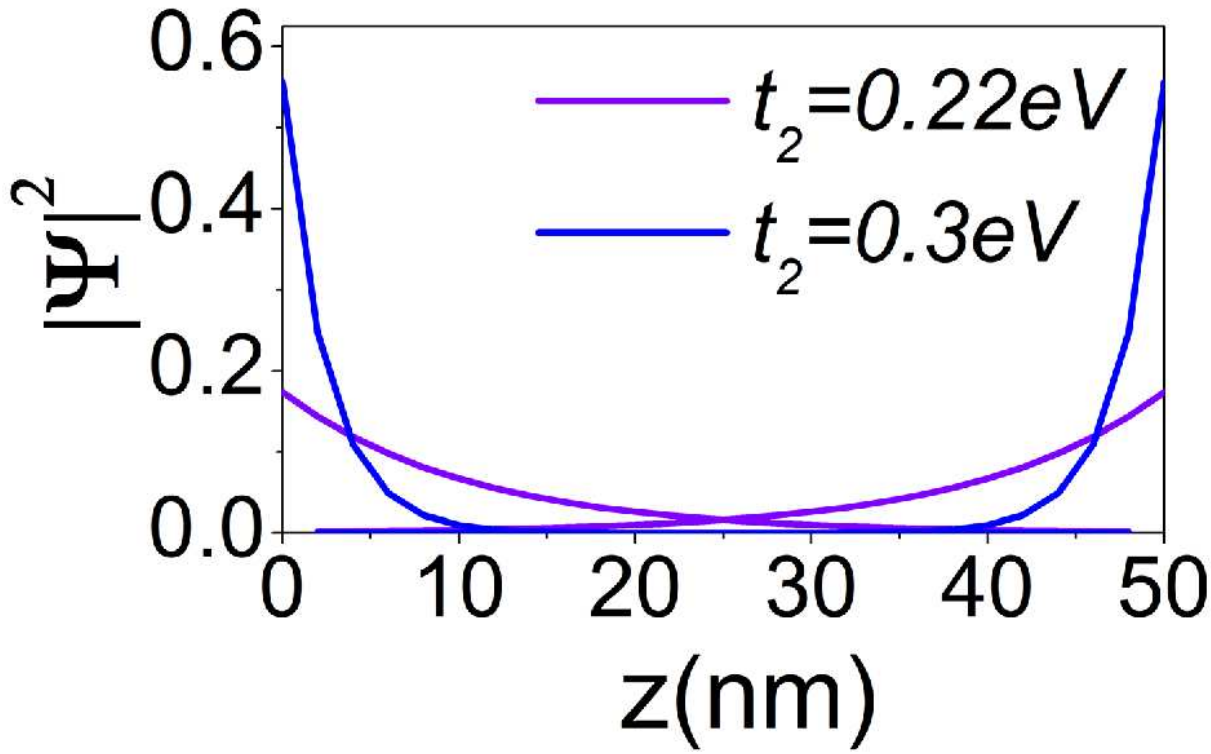
In addition, there are states at the top and bottom surfaces if $t_1 < t_2$ (topological phase) and no surface states if $t_1 > t_2$.
The surface state penetration depth λ is given by

$$e^{-L/\lambda} = \frac{t_1}{t_2}$$

As the temperature increases, t_2 increases and λ decreases as observed experimentally

Hence the two surfaces become more decoupled and the system goes deeper into the topological phase with increasing temperature !

Surface states



Wave functions of surface states for $t_2 = 0.22$ and 0.3 eV, with fixed $t_1 = 0.2$

Hybridization of surface states

If the two surfaces are well separated, the surface states have the dispersion $E_{\vec{k}\pm} = \hbar v_F \sqrt{k_x^2 + k_y^2}$

For a finite separation between the surfaces, the states will hybridize and we get

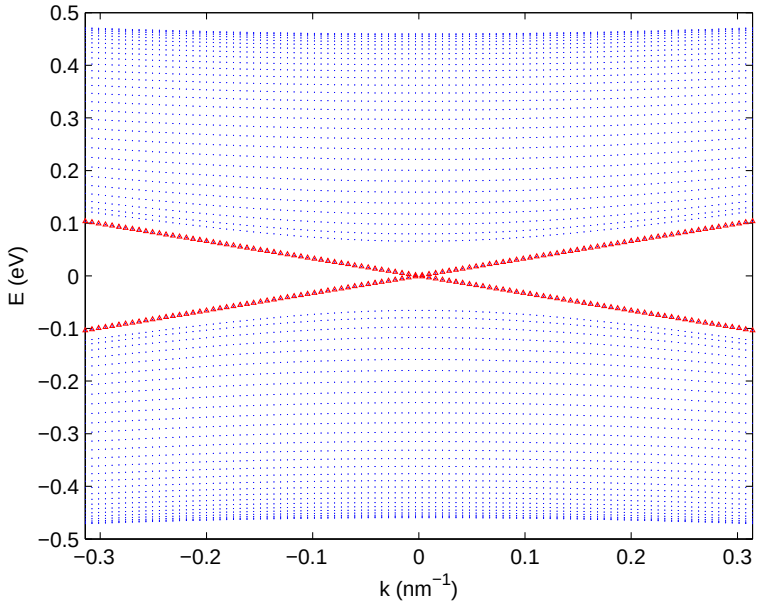
$$E_{\vec{k}\pm} = \pm \sqrt{\hbar^2 v_F^2 (k_x^2 + k_y^2) + \gamma^2}$$

where the gap γ is

$$\gamma \simeq t_2 \left(1 - \frac{t_1^2}{t_2^2}\right) \left(\frac{t_1}{t_2}\right)^N$$

N is the number of grains (i.e., the film thickness is NL)

Effective spin-orbit coupling B_{SOC}



Bulk (blue) and surface (red) states for a system with 30 grains, $v_F = 0.333$ eV nm, $t_1 = 0.2$ eV, $t_2 = 0.25$ eV

With increasing film thickness or temperature, the surface gap γ decreases. Since the Fermi energy $E_F = \sqrt{v_F^2 k_F^2 + \gamma^2}$ is fixed by the conduction band bottom of individual grains, $B_{SOC} = v_F k_F$ increases as γ decreases. Hence B_{SOC} increases with film thickness and temperature as observed experimentally

Berry phase

A perpendicular magnetic field changes the surface state dispersion

$$E_{\vec{k},j} \;=\; \pm\sqrt{\hbar^2 v_F^2(k_x^2+k_y^2)\;+\;(b_z\pm\gamma)^2}$$

where $b_z = (g\mu_B/2)B_\perp$

The Berry phase of one these sets of states with wave function $\Psi_{\vec{k},j}$ is given by an integral around a contour of constant energy. Writing $k_x = k_F\cos\theta,\; k_y = k_F\sin\theta,$ we find the Berry phase to be

$$\begin{aligned}\Phi_j &= -i\int_0^{2\pi} d\theta\;\Psi^\dagger_{\vec{k},j}(k_F,\theta)\;\frac{\partial\Psi_{\vec{k},j}(k_F,\theta)}{\partial\theta}\\ &= \pi\left(1\;\pm\;\frac{b_z\pm\gamma}{\sqrt{\hbar^2 v_F^2 k_F^2+(b_z\pm\gamma)^2}}\right)\end{aligned}$$

As expected, the Berry phase approaches π when $\gamma,\; b_z \;\rightarrow\; 0$

Effect of Zeeman coupling

Berry phase

$$\Phi_j = \pi \left(1 \pm \frac{b_z \pm \gamma}{\sqrt{\hbar^2 v_F^2 k_F^2 + (b_z \pm \gamma)^2}} \right)$$

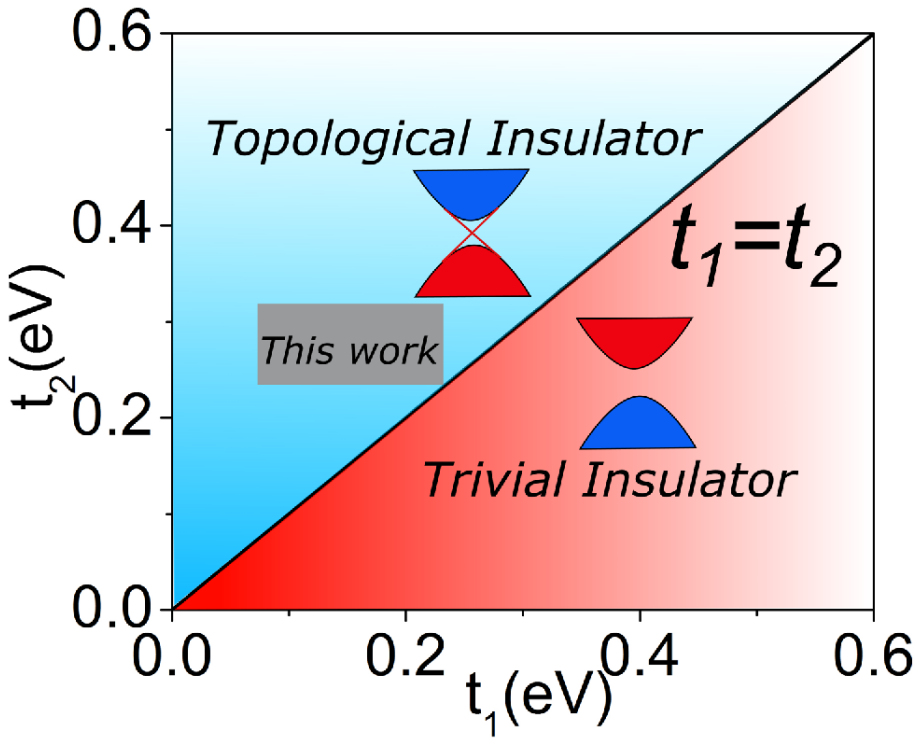
Assuming the surface hybridization γ to be small, the change in the Berry phase due to the Zeeman field leads to the modified HLN formula quoted earlier

$$\begin{aligned} \Delta\sigma_\perp(B_\perp) &= \alpha_\perp \left[1 - 2(B_\perp/B_{SOC})^2\right] \frac{e^2}{2\pi^2\hbar} \\ &\times \left[\psi\left(\frac{1}{2} + \frac{\hbar}{4el_\phi^2 B_\perp}\right) - \ln\left(\frac{\hbar}{4el_\phi^2 B_\perp}\right)\right] \end{aligned}$$

Summary

- We have found that a thin film of coupled TI nanocrystals can have a topological phase like a single crystal of a TI
- The surface state penetration depth is much larger than in a single TI crystal and can be controlled by temperature. The penetration depth decreases and the system becomes more topological with increasing temperature
- The effective spin-orbit coupling (25 - 50 Tesla) is much smaller than in a single TI crystal (several hundred Teslas), and can be controlled by temperature. We have observed an evolution of the Berry phase with the Zeeman field

Summary



Topological phase diagram as a function of intra-grain and inter-grain couplings t_1 and t_2. Our thin film systems are topological insulators but lie close to the phase transition line

Banerjee, Deb, Majhi, Ganesan, Sen and Anil Kumar, arXiv:1604.03767