Заседание Научного Совета РАН «Квантовые технологии»
по теме «Квантовые материалы»

Топологические изоляторы: от идеализированных моделей к реальным материалам

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23 июня 2022 г., Москва

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Preliminary

TI is a material with time reversal symmetry and topologically protected surface states, which continuously connect bulk conduction and valence bands. TI has an energy gap in the bulk interior, just as in an ordinary insulator, but it contains conducting states lon its surface.

An odd number of surface states connects conduction band with valence bands, and crossings at time-reversal-invariant points in Brillouin zone (Dirac points), which leads to topologically *protected* metallic boundary states.

The main ingredient is the existence of spin-orbit coupling, which can be understood as a momentum-dependent magnetic field coupling to the spin of the electron.

OUTLINE

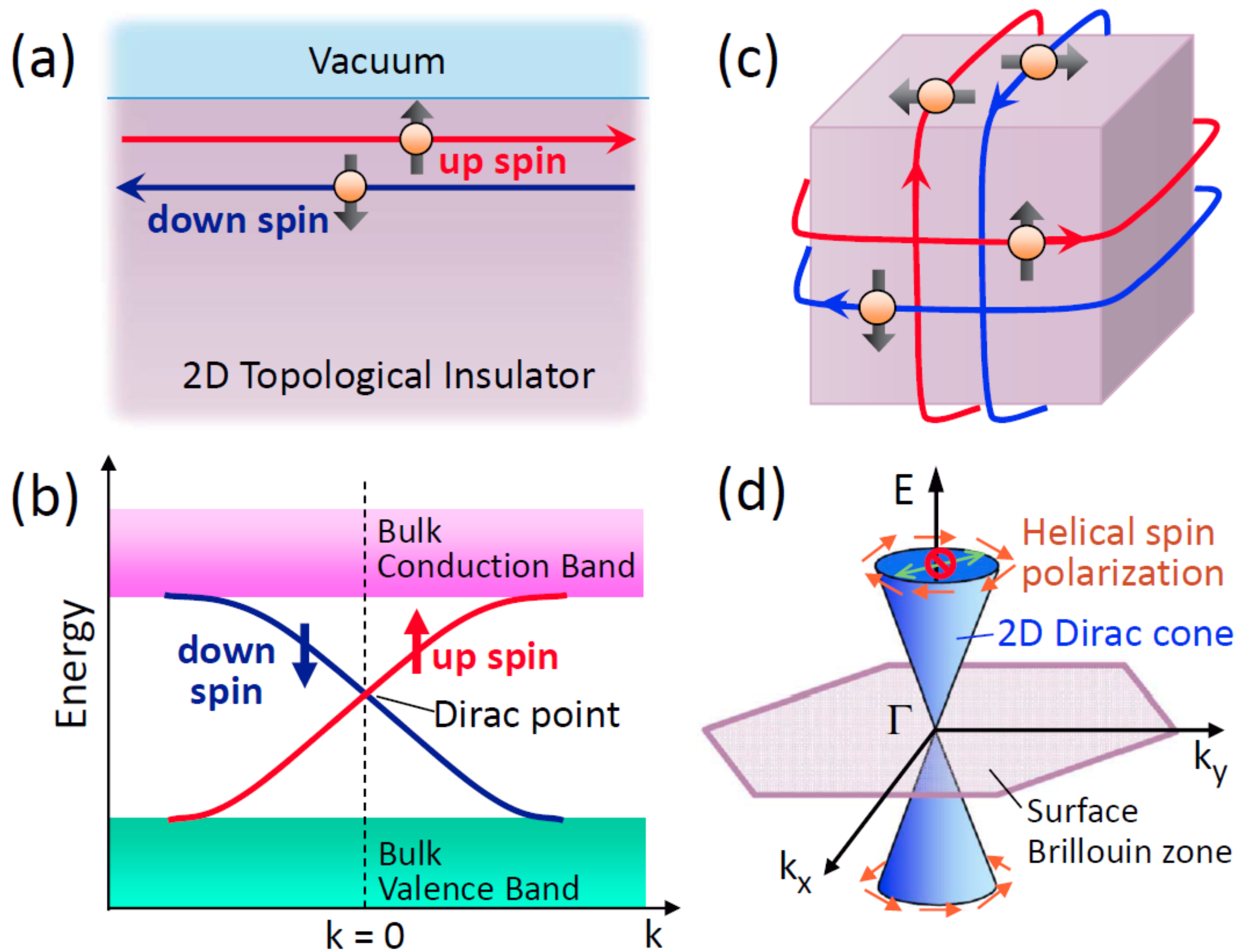
- **Introduction**
  - Basic models for TI
  - Spin-momentum locking
  - Absence of backscattering
- **From ideal models to real systems**
  - The emergence of backscattering
  - The failures for 2D TI
- **The study of BSSTS – the best 3D TI**
  - Main properties and band structure
  - ESR studies
  - Nanosize charge droplets in a bulk
- **Conclusions**

Publications

[1] V. Sakhin, E. Kukovitsky, Yu. Talanov, G. Teitel'baum, JETP Letters, 113:4 (2021), 273–278.

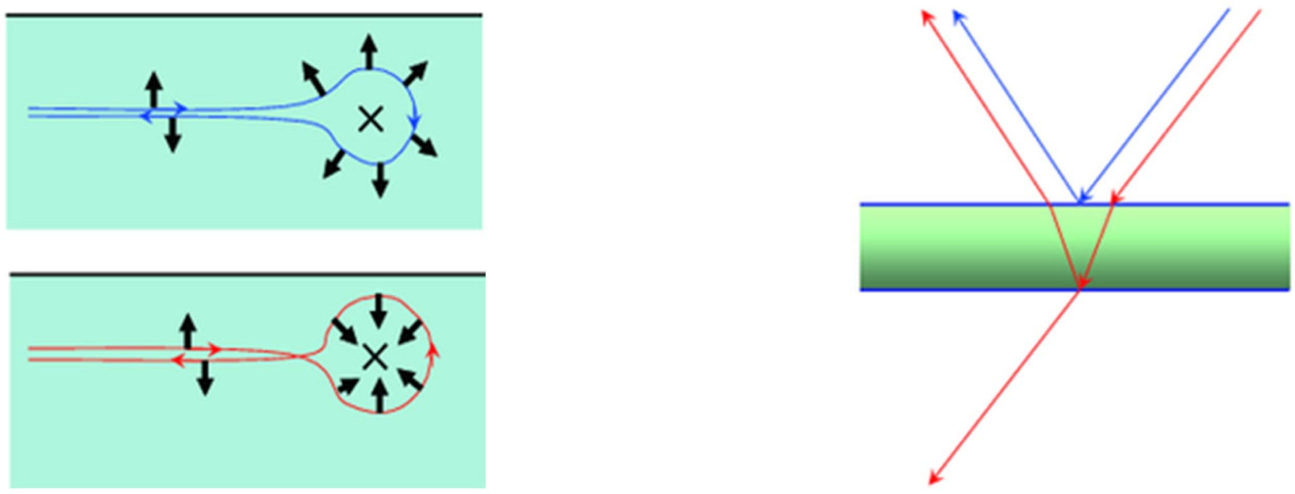
[2] V. Sakhin, E. Kukovitsky, Yu. Talanov, G. Teitel’baum, L. Morgun, A. Borisov, A. Usoltsev, and V. Pudalov, JETP Letters, Vol. 115:4 (2022), 239–244.

2D and 3D Topological insulators



Spin-momentum locking and absence of back scattering

Absence of backscattering



(a) (b)

(a) A quantum spin Hall edge state can be scattered by a nonmagnetic impurity clockwise (spin rotates by π) or counterclockwise by −π. A quantum mechanical phase factor of −1 associated with that difference of 2π leads to destructive interference of two paths---backscattering of electrons is suppressed in a way similar to that of photons off the antireflection coating.

(b) On a lens with antireflection coating, light waves reflected by top (blue line) and bottom (red line) surfaces interfere destructively, which leads to suppressed reflection.

Magnetic impurities destroy this picture!

Attractive features and applications

- Topological stability
- Spin-momentum locking
- No back scattering

- Reliable devices
- Spintronic applications
- Spin-charge conversion
- High mobility

Introduction

Historical comment

Pankratov, O.A.; Pakhomov, S.V.; Volkov, B.A. (January 1987). "Supersymmetry in heterojunctions: Band-inverting contact on the basis of Pb1-xSnxTe and Hg1-xCdxTe". Solid State Communications. 61 (2): 93–96.

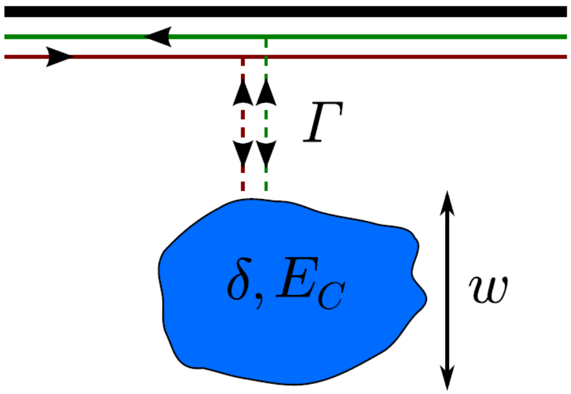
Bibcode:1987SSCom..61...93P. doi:10.1016/0038-1098(87)90934-3

M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann L.W., Molenkamp, X.-L. Qi, and S.-C. Zhang, HgTe/(Hg,Cd)Te quantum wells, Science 318, 5851 (2007).

For 2D TI, when the Fermi level resides in the bulk gap, the conduction is dominated by the edge channels that cross the gap. The two-terminal conductance is $G_{xx}=2e^2/h$ and its value of the conductance should be insensitive to the width of the sample.

This is true only in assumption that region between conducting surfaces or edges is a uniform insulator, and local inhomogeneities of charge distribution in this region may be neglected.

However, real substances always contain such inhomogeneities. For 2D TI electrons moving along a helical edge tunnel in and out of puddles created by the inhomogeneous charge distribution in the vicinity of this edge. In the puddles, electrons may undergo inelastic backscattering



A quantum dot of linear size w tunnel-coupled to a helical edge. The mean level spacing of puddle is denoted by δ and its charging energy by E_C. The typical tunneling-induced level width is Γ.

[1] “Helical Edge Resistance Introduced by Charge Puddles”, J. I. Väyrynen, M. Goldstein, and L. I. Glazman. , Phys. Rev. Lett. 110, 216402 (2013).

[2] “Resistance of helical edges formed in a semiconductor heterostructure”, J. I. Väyrynen, M. Goldstein, Y. Gefen, and L. I. Glazman., Phys. Rev. B 90, 115309 (2014).

[3] "Failure of conductance quantization in two-dimensional topological insulators due to non-magnetic impurities” Pietro Novelli, Fabio Taddei, Andre K. Geim, and Marco Polini, Phys. Rev. Lett. 122, 016601 (2019)

[4] “Current Noise from a Magnetic Moment in a Helical Edge” Jukka I. Väyrynen and Leonid I. Glazman., PRL 118, 106802 (2017)

[5] “Unrestricted Electron Bunching at the Helical Edge” Pavel D. Kurilovich, Vladislav D. Kurilovich, Igor S. Burmistrov, Yuval Gefen, and Moshe Goldstein., Phys. Rev. Lett. 123, (2019) 056803.

An important issue is the detection and analysis of similar inhomogeneities in real three-dimensional TIs, where their presence seems also to be very probable. The fact is that complete suppression of bulk conductivity in them is achieved by compensating for current carriers by adding to their structure a small amount of impurity ions - donors, in the case when it is necessary to "neutralize" holes or acceptors when it comes to "neutralizing" electrons. As a result, charged defects appear in the structure giving rise to local distortions of the band gap, which are anomalously strong when the screening is suppressed due to the small number of current carriers.

In this regard, the role of various local methods in studying the properties of TI has significantly increased. One of the promising tools for solving such problems is spin resonance of current carriers (ESR) which can be used to study local inhomogeneities in the distribution of charge and spin excitations.

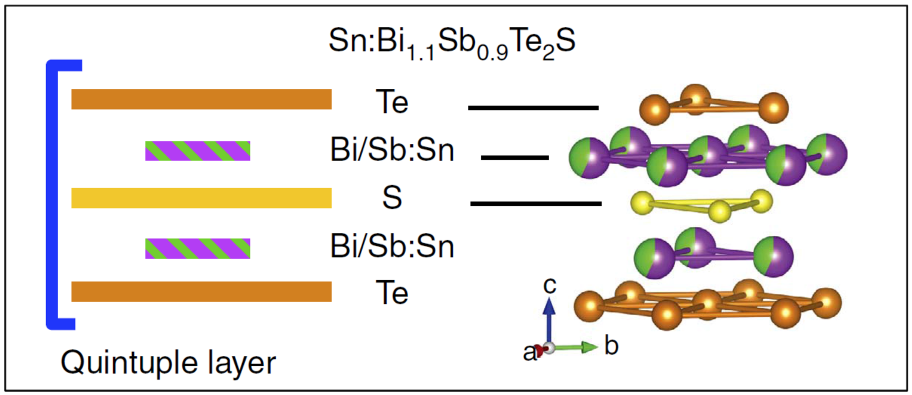
This problem requires serious research!

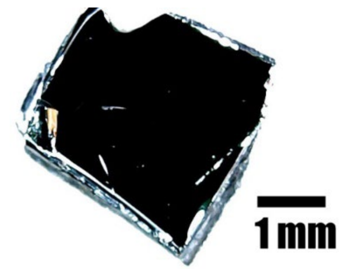
BSSTS

$Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$

$Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$

One of the best 3D topological insulators



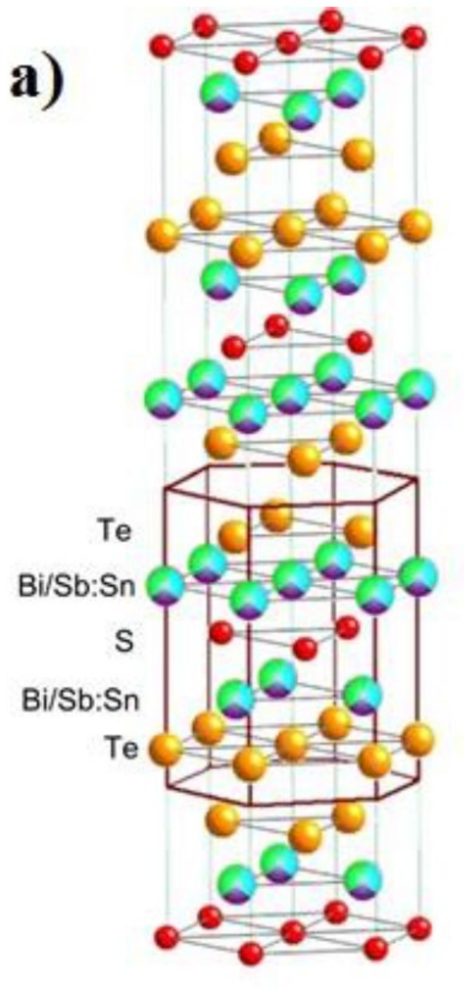


Single crystals were grown in our group using technology published in:

Kushwaha, S. K. et al. Nat. Commun. 7:11456
doi: 10.1038/ncomms11456 (2016).

Additional elements: Stanum, Sulfur, Stibium

$Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$



X-ray

$Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$

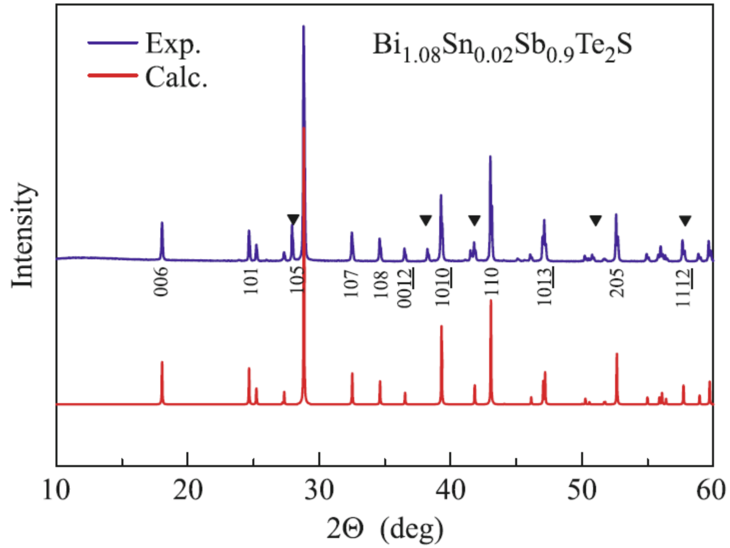
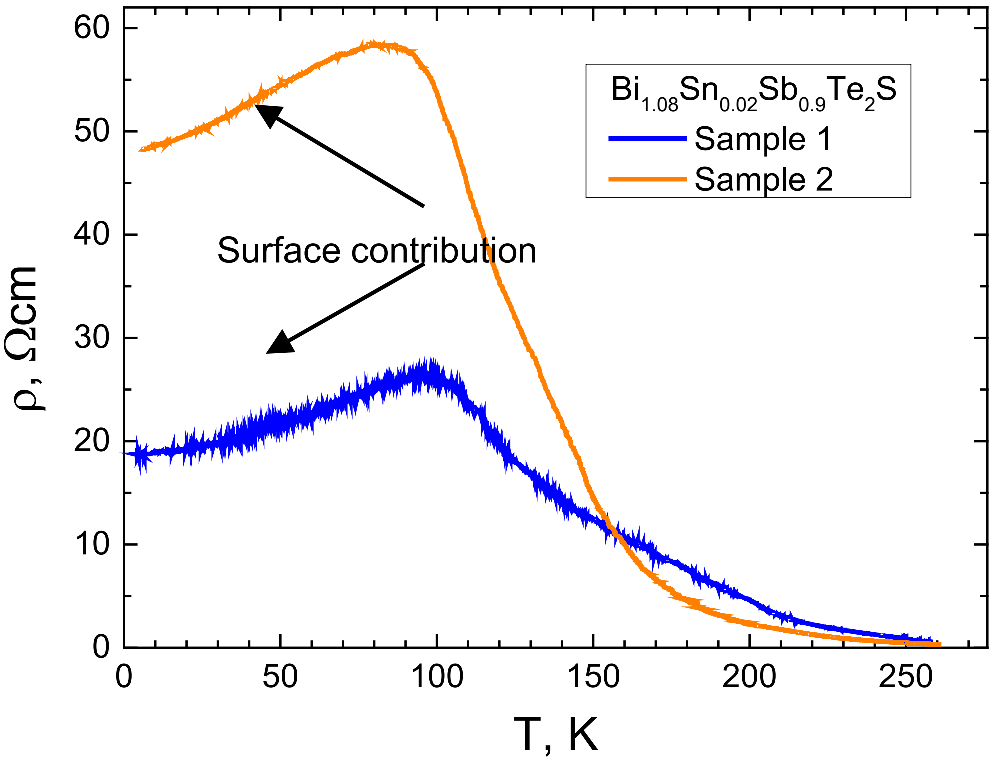


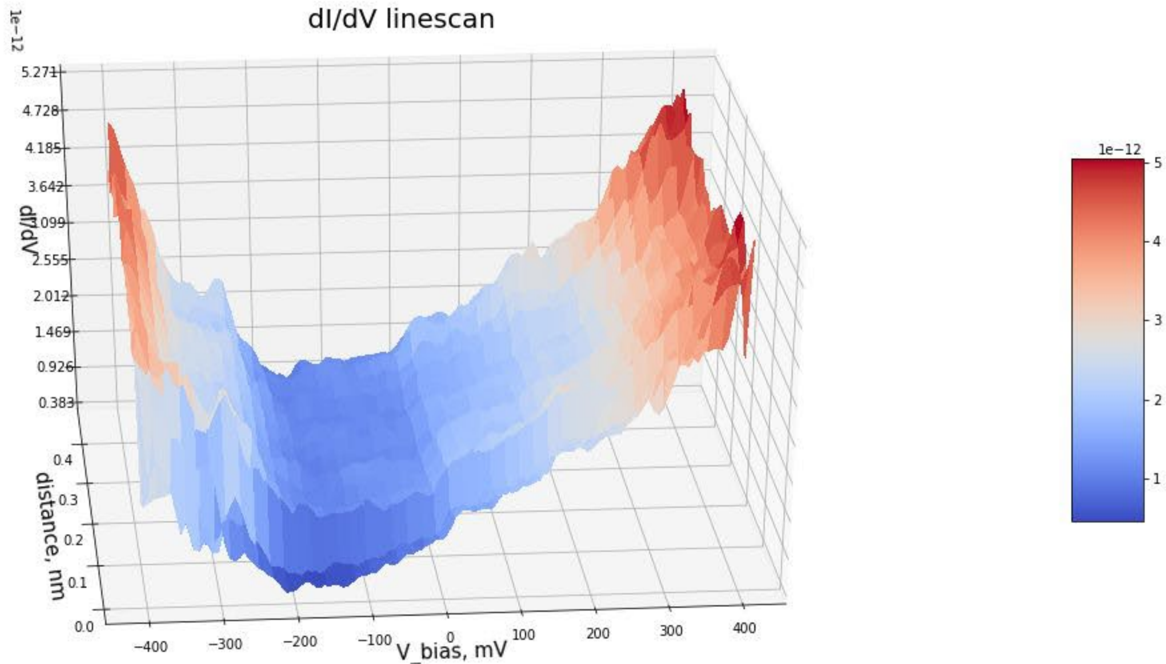
Fig. 1. (Color online) X-ray diffraction pattern of the $Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$ sample grinded into a powder (upper line). Weak reflections related to the spurious $BiSbTe_3$ precipitated phase [14] are marked by triangles (see the text for details). The lower line corresponds to a diffraction pattern calculated using the POWDER CELL program [13].

Resistivity

$Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$



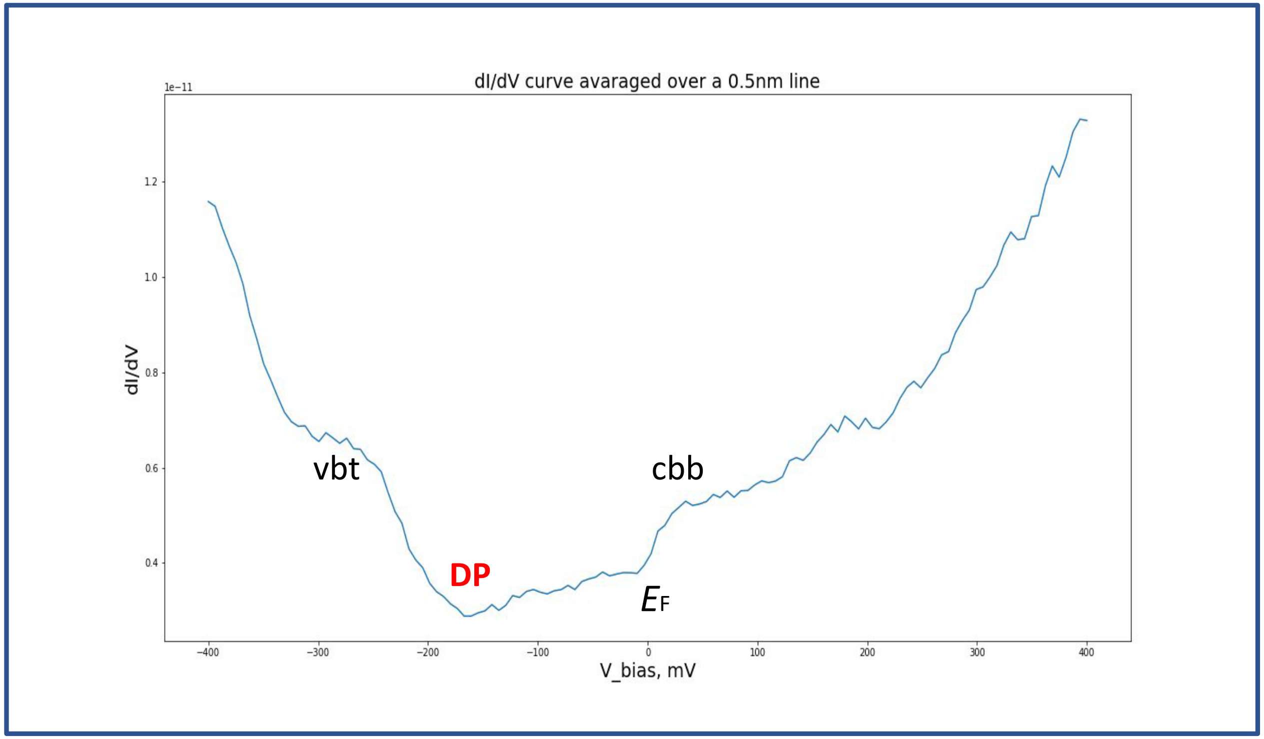
dI/dV line scan

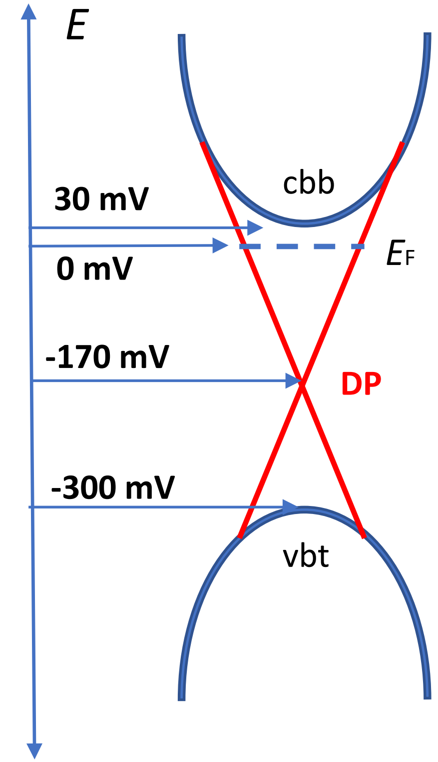


Ultra low temperature and high magnetic field STM Unisoku (T=2K)

Band structure

$Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$



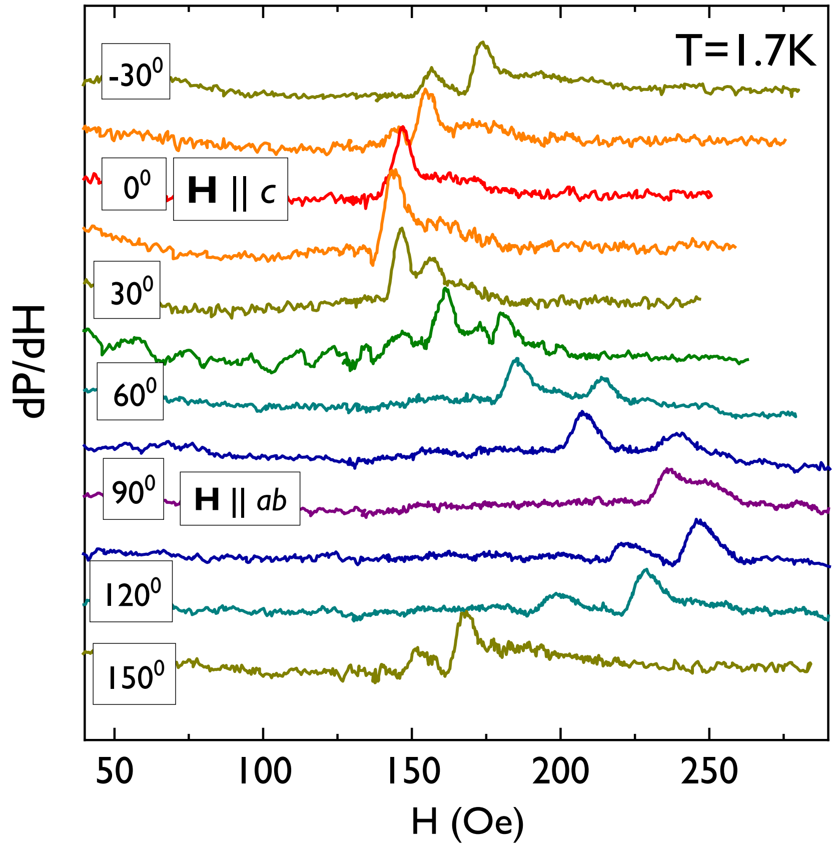


Ultra low temperature and high magnetic field STM Unisoku (T=2K)

Band structure
Kukovitsky, 2019

ESR angular dependence

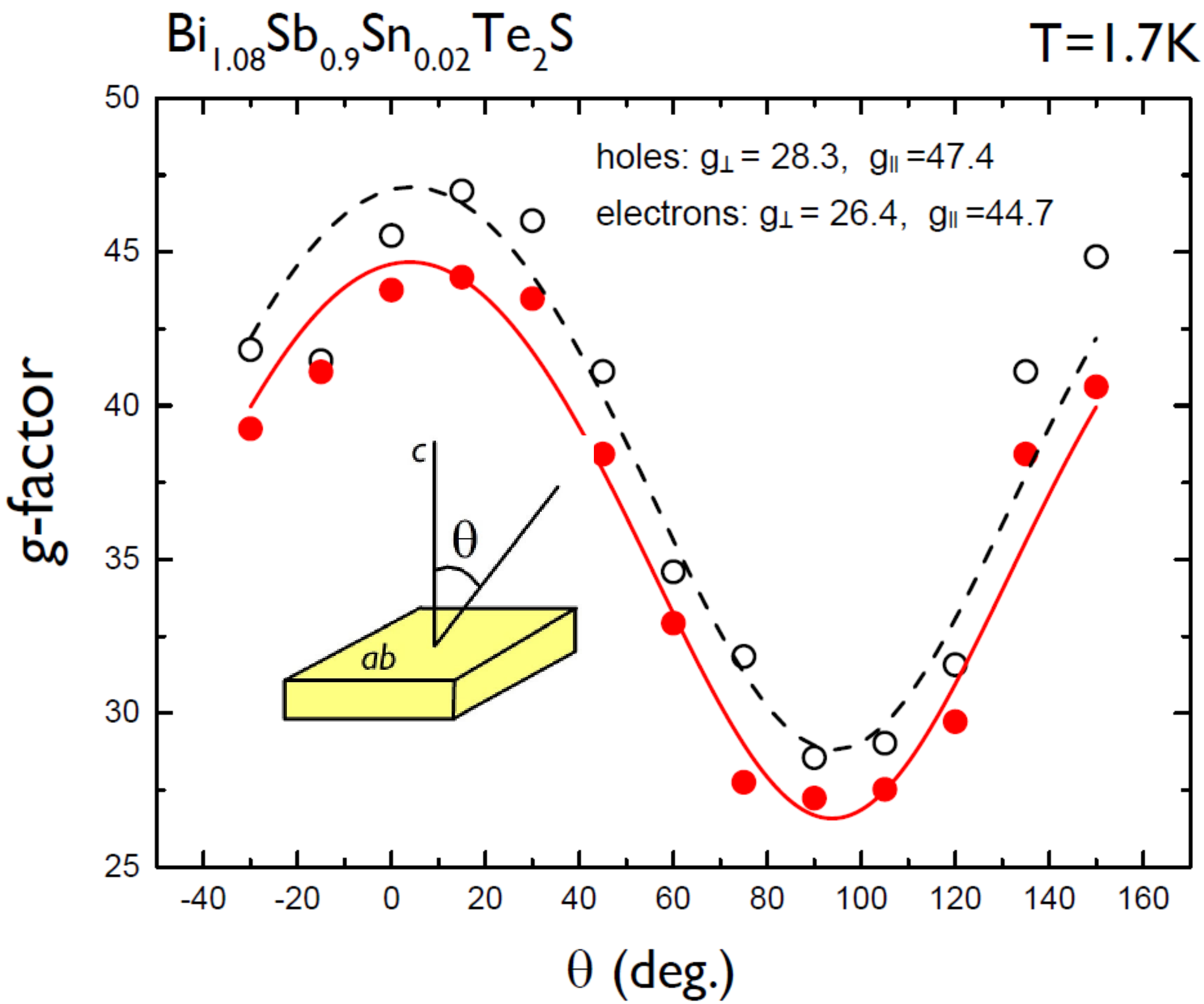
$Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$



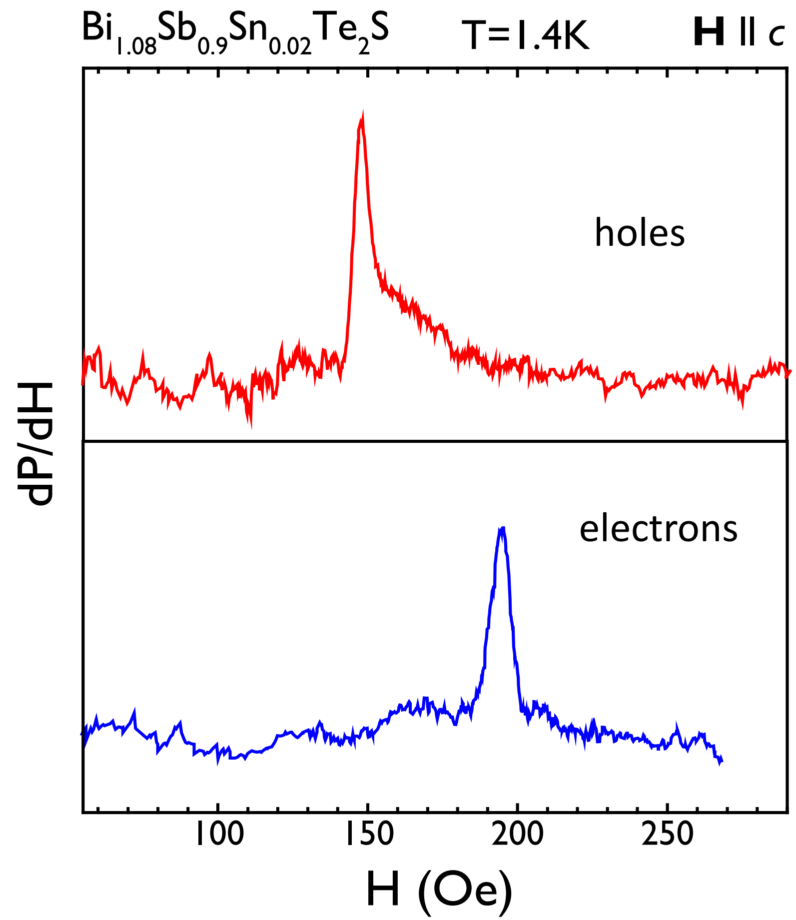
X-band ESR

Superposition of two ESR lines with large g-factors

g-factor angular dependence



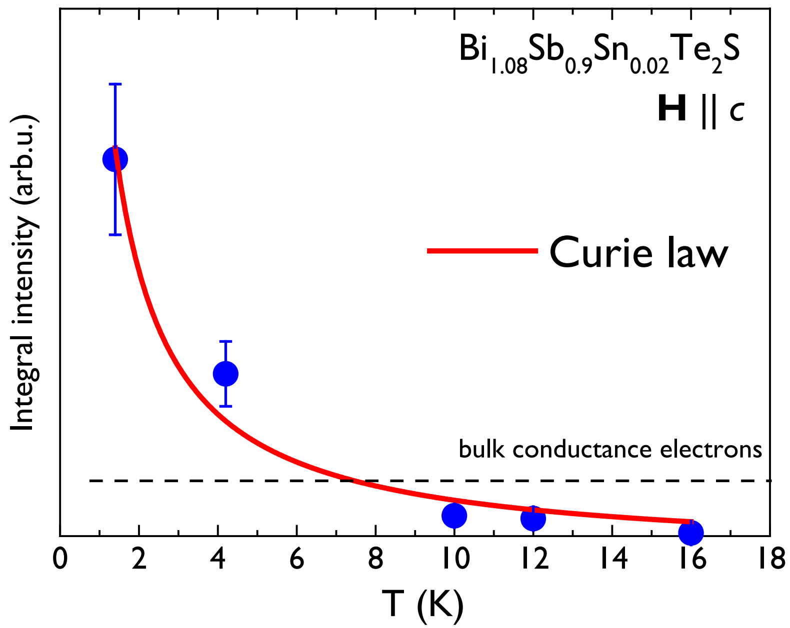
ESR of holes and electrons



X-band ESR

ESR integral intensity

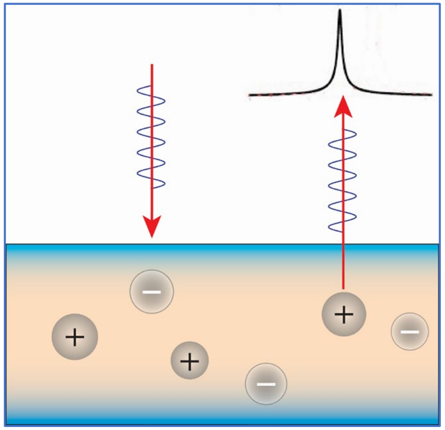
Small metallic particles?



Temperature dependence of integral intensity is not corresponding to Pauli law, but to Curie law (~1/T).

It is characteristic feature of small metallic particles with quantized energy spectrum, where distance between levels is larger than kT.

(L.P. Gor'kov, G.M. Eliashberg, JETP 1965)



ESR of small metallic droplets !?

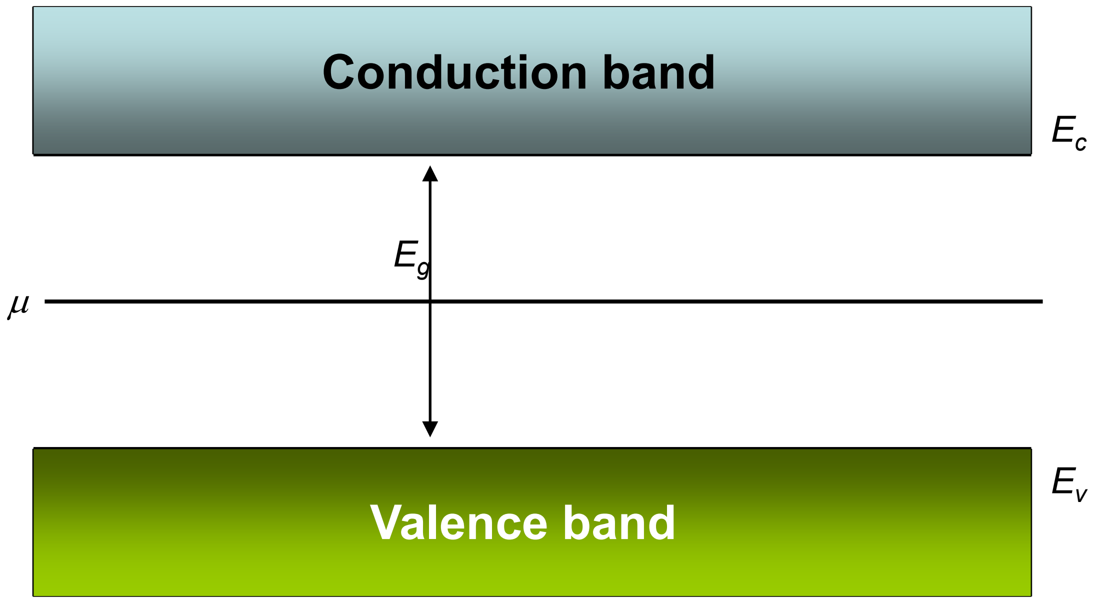
Nanosize metallic particles (droplets)

- Density of states for small particles $\nu = Vm^* p_0/2\pi^2$
- $V \sim a^3$ – particles volume
- Average distance between energy levels $\Delta = 1/\nu$ is finite and depends on V
  (L.P. Gor'kov, G.M. Eliashberg, JETP 48, 1407 (1965))
- For $\Delta < kT$ susceptibility is of Pauli type
- For $\Delta > kT$ susceptibility is of Curie type
- The crossover temperature may be used for estimation of typical size of metallic particles ($a \sim$ several nanometers)

Nanosize charge droplets

No bulk conductivity

The expected band structure in the absence of bulk conductivity



What for $Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$ case?

Nanosize charge droplets

No bulk conductivity

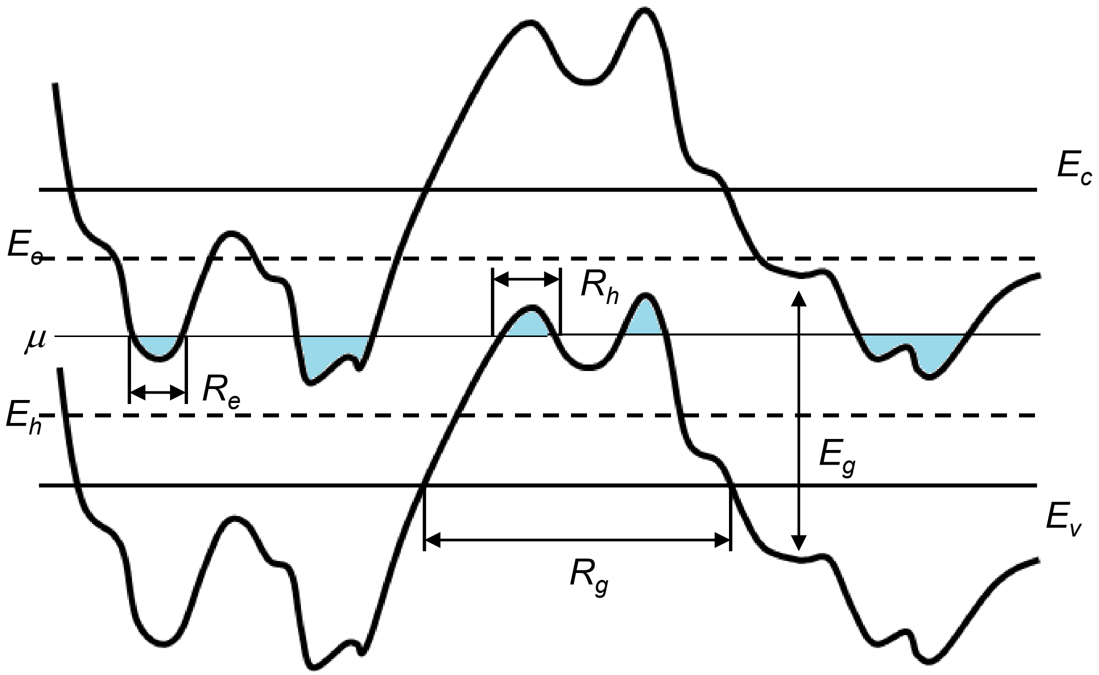
- Complete suppression of bulk conductivity is achieved by compensating for current carriers by adding to their structure a small amount of impurity ions - donors, in the case when it is necessary to "neutralize" holes or acceptors when it comes to "neutralizing" electrons.

- In this case, charged defects appear in the structure, which leads to local distortions of the band gap, which are anomalously strong at a weakening of the screening characteristic of a small number of carriers.

- This circumstance can lead to the appearance of peculiar nanosized charge droplets in the sample volume.

Space variation of the band gap

Nanosize droplets $R_e \sim R_h \sim 10$ nm



B.I. Shklovskii A.L. Efros. Electronic Properties of Doped Semiconductors. Springer-Verlag. 1984.

Summary

- Using ESR, the formation of nanosized charge "droplets" in the Bi1.08Sn0.02Sb0.9Te2S volume was detected. Droplets located near the surface may be the reason of inelastic backscattering

- Since the electrons and holes are "locked" in these droplets their participation in the conductivity by ordinary charge transfer is impossible. At relatively high temperatures, the bulk conductivity is of an activation nature, with activation energies that can be much less than half the band gap due to percolation.

- At sufficiently low temperatures, electrons and holes tunnel between droplets, and thermally activated transport is replaced by variable-length hops.

- The results obtained can be used for the correct interpretation of transport in real single crystals, as well as for the targeted synthesis of new TIs.