Topological Insulator Materials and Nanostructures for Future Electronics, Spintronics and Energy Conversion

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***Abstract* – Two fundamental electrons attributes in materials and nanostructures - charge and spin – determine their electronic properties. The processing of information in conventional electronic devices is based only on the charge of the electrons. Spin electronics, or spintronics, uses the spin of electrons, as well as their charge, to process information. Metals, semiconductors and insulators are the basic materials that constitute the components of electronic devices, and these have been transforming all aspects of society for over a century. In contrast, magnetic metals, half-metals, magnetic semiconductors, dilute magnetic semiconductors and magnetic insulators are the materials that will form the basis for spintronic devices. Materials with topological band structure attributes and having a zero-energy band gap surface states are a special class of these materials that exhibit some fascinating and superior electronic properties compared to conventional materials allowing to combine both charge and spin functionalities. This article reviews a range of topological insulator materials and nanostructures with tunable surface states, focusing on nanolayered and nanowire like structures. These materials and nanostructures all have intriguing physical properties and numerous potential practical applications in spintronics, electronics, optics and sensors.**

***Index Terms* – Topological insulator, nanowire, nanoribbon, bismuth selenide, magnetotransport, metal-insulator transition, , structure interfaces, thin film.**

I. INTRODUCTION

Depending on the electronic band structure and transport characteristics uncountable number of materials and substances can be classified quite simply in terms of their conductive behavior into one of three types — insulators, semiconductors and metals. More than three decade ago there was established that spin-orbit interaction (SOI) has an important pattern on band structure of solid state matter. Among different qualitative features induced by SOI the band inversion of electronic spectrum near the Fermi level has been discovered. Such type of electronic spectrum was identified in different type of semimetalic and narrow-gap semiconductors $Bi_{1-x}Sb_x$, $Pb_{1-x}Sn_xTe$, Bi_2Te_3, HgTe, $TlBiTe_2$ etc. In the context of low dimensional structure investigations the band spectrum inversion was shown to generate new type of interface gapless states with linear spectrum at the heterocontact boundaries. Last years investigations [1,2] have reopened the interest to materials with inverted band spectra. Due to new type of the symmetry break like that characteristic for the integer and fractional quantum Hall effects the electronic states was shown to have topological nature and materials have been named toplogical insulators (TI) (Fig.1). Thus in TI a new state of matter appear, distinguished from a regular band insulator by a nontrivial time-reversal topological invariant, which characterizes its band structure, and non-trivial interplay of charge and spin degree of freedom of band electrons. In results new physics and phenomena related to this states have greatly emerged. Several of such new TI properties are reviewed in the paper as well as some old observed properties of materials with band inversion. Many intriguing properties of TI can be ascribed to the existence of two-band gaplees Dirac electrons in its low-energy band structure. Actually, Dirac electrons with finit gap in materials have a long history starting from bismuth that has three-dimensional massive Dirac electrons in its band structure

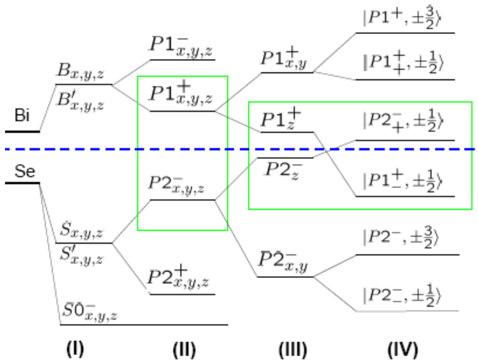

Fig.1. Band spectrum inversion – the origin of genesis of the topological insulator state

The most robust observable consequence of a nontrivial topological character of these materials is the presence of gapless helical edge states (interface states of inverted heterocontacts), whose gapless states is protected by time-reversal symmetry and is thus robust to perturbations that do not break this symmetry (Fig.2). Like the Hall state the “bulk” of the electron gas of TI is an insulator, but along its suface, the states can be gapless. Within a certain parameter range the surface states of TI are well described by a Dirac cone, allowing for parallels with graphene and relativistic physics, and prohibiting backscattering.. A prerequisite for such experiments is a highly tunable surface state which is decoupled from the residual bulk carriers. Despite considerable recent evidence of TI surface states in ARPES and STM , transport experiments are complicateddue to significant parallel conduction through bulk states, limited surface density tunability, and uncertainty of the surface to bulk coupling. At the same time the spectrum and characteristics of topological surface states (TSS) depending on geometrical configuration can be manipulates by different factors: electrical and magnetic fields, strain and deformation ets. For this reason TI are being explored with a view towards applications, as a potential platform for tailoring nanostructures and nanomaterials properties. This topics cover the second part of the paper.

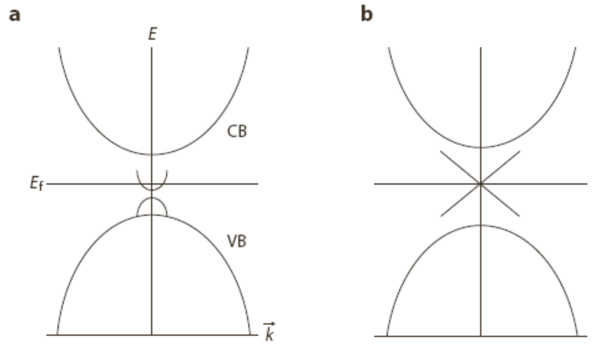

Fig.2 The electronic band structures of topological insulators, a new class of quantum matter with (a) a robust metallic state at the surface/edge and insulatingproperties in the bulk/surface, and (b) a conductive state at the surface or edge withzero gap and the same linear energy dispersion as graphene.

The last part of the paper deals with behavior of TSS if TI nanostructures in the nanowire and nanotube like configuration Some aspects of transport through TSS are discussed: anomalous Aharonov-Bohm conductance oscillations; magnetic quantum oscillations, edge accumulation and currents of moment.Thermoelectric aspect of TSS are discussed in the context of TI materials Bi_2Se_3 and Bi_2Te_3 knowing as the best thermoelectrics.

II. TOPOLOGICAL INSULATOR NANOLAYERED STRUCTURES

Along with the extensive researches of materials and properties of three- dimensional (3D) topological insulators (TIs),[1] attention has increasingly been paid on ultrathin films and nanostructures of such materials for enhanced effects and properties associated with the topological states of electrons [2,3] In the same line of thoughts, multi-layered structures constituted of TIs and normal band insulators, such as superlattices (SLs) or multiple quantum well (MQWs) of …Bi2Se3/ZnSe…have been attempted by the technique of molecular-beam epitaxy (MBE). In this part of paper we are using formal analogy of electromagnetic wave equation and Schrodinger equationin order to study the phenomenon of perfect tunneling (tunneling with unitary transmittance) in multilayered semiconductor heterostructure with band inversion and TSS. Using the two-band model of semiconductor we are showingthat such phenomenon can indeed exist, resembling all the interesting features of the analogous phenomenon in classical electromagnetism in which metamaterials (substances with negative materialparameters) are involved. We believe that these results can open up the way to interesting applications in which the metamaterial ideas are transfered into semiconductor domain.

The evolution of the topological states in dependence of layer thickness and others factors are highlighted for quantun well and superlattice structures based on $Bi_{1-x}Sb_x$, Pb1-xSnxTe, Bi2Te3 in the framework of two-band effective mass method. In the superlattice structures like PbTe/SnTe with layer thickness a and b respectively the state of the topological insulator can be realized (Fig.3).

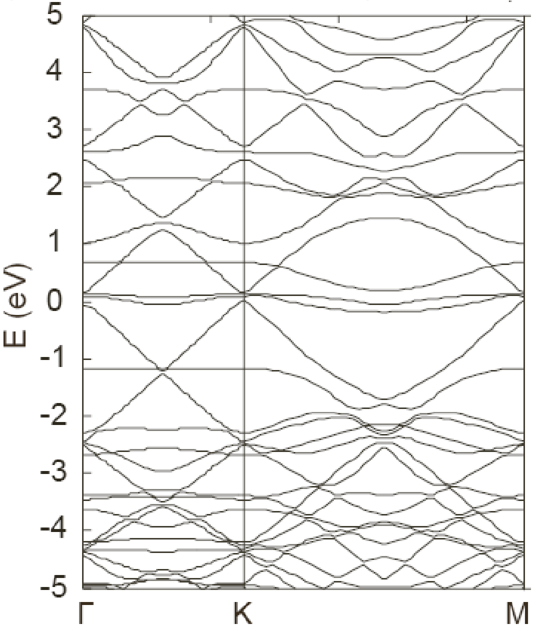

Fig.3. Topological extended states in PbTe/SnTe superlattice structures

The dispersion relation E(K), K being the crystal momentum, can be found from [4]

$$\cos q(a+b) = \cosh(Kb)\cos(ka) - [(p^2 - r^2)/2pr]\sinh(Kb)\sin(ka).$$

Where $k==(E^2 - E^2gA/4)^{1/2}/hv$,

$K==(E^2gB/4 - E + V)^{1/2}/hv$,

$r =(E - EgA)/2hvk$,

$p=(EgB/2 - E + V))/2hvK$

The phase diagram of the band and topological insulator states are established in dependence of the semiconductor gaps and thickness. The gapless electronic states with Dirac like linear spectrum were revealed to occur when $E_{gPbTe} * a = Eg_{SnT}e * b$. Such superlattice structures can be considered as a new type of metamaterial of semiconductor layers and metallic sheets. The plasmonic and metamaterial characteristics of such layered structures are discussed. Flat-lens focusing of electrons on the surface of a topological insulator $B_{i2}Te_3$ is analysed. The early studied interface states in inverted heterocontact with magnetic ordering are reanalyzed in the context of recently discovered antiferromagnetic TI. The occurrence of interface ferromagnetism is demonstrated [5].

III. TUNABLE TOPOLOGICAL STATERS IN NANOWIRES

The surface contribution is easier to extract experimentally in TI nanowires , where the surface-to-volume ratio is more advantageous. In this case, introduction of a magnetic flux piercing the nanowire has allowed to successfully identify the Aharonov-Bohm effect caused by the surface state.

The TSS of cylindrical nanowires and topological insulator Bi2Te3 with cylindrical pores are studied. The developed recently low-energy approach for bulk Bi2Te3 is used to highlight TSS on the cylindrical surface. For the bulk

Bi2Te3 (Bi2Se3) TI near the Γ point of the surface Brilloiun zone, Hamiltonian has the form

$$H = \varepsilon_0(\mathbf{k})\sigma_0\tau_0 + M(\mathbf{k})\sigma_0\tau_z + A_1 k_z \sigma_z \tau_x + A_2 \tau_x (k_x\sigma_x + k_y\sigma_y).$$

Model parameters of four bands Hamiltonian (1) have been defined in the framework of kp theory by comparison with the ab initio calculations [7].

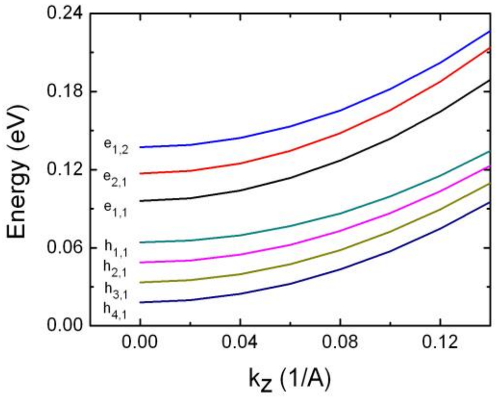

Fig.4. Electronic structure of TI Bi2Te3 nanowire with a radius of 10 nm.

The TSS forming inside the bulk gap (Fig.4) corresponds to one dimensional bands indexed by total angular momentum. For nanowire or nanopore of radius R, the wavefunction to vanish at the boundary r = R is required, which is automatically ensured by expanding in the orthonormal set of radial Bessel functions Jm or Ym with integer m. In comparison with gapless character os TSS of flat surface all TSS modes of cylindrical surface have a finite gap described qualitatively by relations Egs ~v/R (Fig.5). In results nanowire and nanopore composites of TI have distinct from layered ones pecularities and several are discussed in the paper [8]

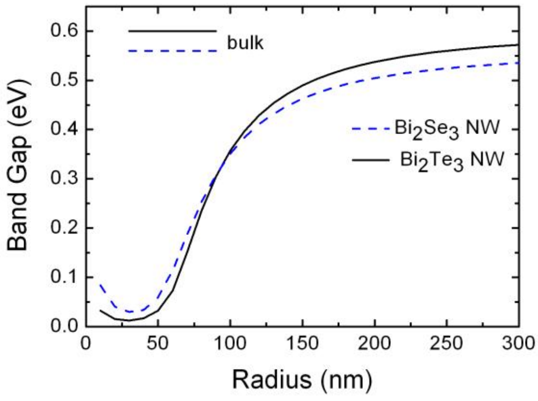

Fig.5 Dependence of the direct band gap at the Γ point of the topological insulator Bie2Te3 (solid line) and Bi2Se3 (dashed line) nanowires on radius.

IV. TOPOLOGICAL INSULATOR NANOSTRUCTURES AND ENHANCED THERMOELECTRICAL PERFORMANCE

Last years investigations of new electronic states of materials and structures - topological states - as well as new physics and phenomena related to this states, which are generated by new type of the symmetry break like that characteristic for the integer and fractional quantum Hall effects, have greatly emerged. In the Hall state the “bulk” of the electron gas is an insulator, but along its edge, electrons circulate in a direction that depends on the orientation of the magnetic field and these edge states are different from ordinary states of matter because they persist even in the presence of impurities. Recently it was established that the same “robust” conducting edge states could be found on the boundary band insulators with large spin-orbit effect, called topological insulators. In a topological insulator (TI), these surface states are protected, that is, their existence does not depend on how the surface is cut or distorted. Such type of topological states and its related effects (in particular quantum spin Hall effect) are analized for different type of semimetalic and narrow-gap semiconductor materials Bi1-xSbx, Pb1-xSnxTe, Bi2Te3, HgTe and their nanostructures.

Recent photoemission experiments reveal that Bi_2Te_3 and other like termoelectrics are a TI with a single Dirac cone on the surface, consistent with electronic structure predictions. In this part of the paper we try to analyze how new surface topological states could lead to improved thermoelectric performance. The physical system to be studied here is a thin film and nanowire of Bi2Te3. If the film is thin enough the surface states on both sides hybridize and open a gap [6].

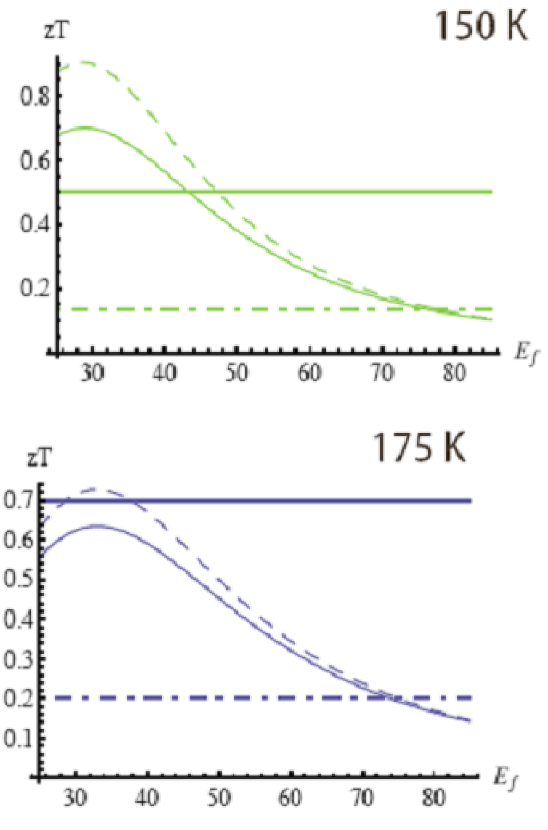

Fig .6. ZT for the thin film including bulk contributions at 150 and 175 Kelvin. The straight line in each figure corresponds to the best known ZT at the same temperature. Dashed line indicates the ZT for the surface states alone and Dashed-Dotted line indicates ZT for bulk Bi2Te3.

Although the film thickness required to open an observable gap for TI surface states (1-10 nm) is small, it is accessible with current growth techniques and very recently the hybridization gap has been observed by in-situ photoemission on thin films of Bi_2Se_3.Using the electron dispersion the in-plane (longitudinal for nanowire) transport coefficients for the surface states together with bulk ones were obtained and calculated as well as for the figure of merit ZT (Fig 8) [9].

As is evident from Fig. 6, at temperatures below 150 K, which are important for several Peltier cooling applications, the thermoelectric performance of the topological insulator thin film is signifcantly enhanced because of the high ZT of the protected edge topological states. At low temperature the bulk contribution is smaller than the surface contribution so that the unknown chemical potential dependence of bulk properties is not too significant. Crucially, the gap in the hybridized surface mode band structure can be controlled by tuning the thickness of the film to get high ZT in a specific temperature range. The geometry of thin films is also very effective in reduction of phonon thermal conductivity, so there will be even larger enhancement for the topological insulator like $B_{i2}Te_3$ thin films. The same approach applies as well to nanowires.

V. CONCLUSIONS

Materials having signature of topological insulator are a special class of materials that exhibit fascinating and superior electronic, magnetic and optical properties compared to conventional materials. The discovery of topological insulator state of matter has generated great interest in the search for new classes of such materials, and some classical materials with band inversion spectra have been revisited. The phase diagram of the band and topological insulator states are established in dependence of the semiconductor gaps and thickness in Ti multilayered structures (materials A and B). The gapless electronic states with Dirac like linear spectrum were revealed to occur when $E_{gA} * a = Eg_B * b$. Such superlattice structures can be considered as a new type of metamaterial of semiconductor layers and metallic sheets.

Analysis of TI nanowires draw a consistent picture for the surface states inside the bulk gap, even for very thin nanowires: a one-dimensional (1D) electron waveguide with modes indexed by the half-integer total angular momentum j is formed, where each mode contains a rightand a left-mover. The spin direction is always tangential to the surface and perpendicular to the momentum.

In the simplest singlemodecase, the spin polarization of a right (left) moverhas a counter-clockwise (clockwise) orientation around the waist of the cylinder.

The cylindrical symmetry leads to a decrease of the band gap with decreasing of both NW radius and ratio bulk volume/surface area, while the confinement effect leads to an increase of the band gap at a rather small value of the NW radius.The observation of the Aharonov-Bohm oscillations in Bi_2Se_3 nanostructures provides important insights into the topological surface states.

The topological states of Bi_2Te_3 thin film surfaces hybridize and band gap is opened. In results, increased thermoelectric performance of film and nanowire can occur at low temperatures. The analyzed results may lead to a new method of improving the thermoelectric figure of merit for more efficient thermal-to electric energy conversion and thermal management of devices.

REFERENCES

[1] Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Nat Phys 5 (6), 398 (2009)
[2] J. G. Checkelsky, Y. S. Hor,R. J. Cava, and N. P. Ong, PRL 106, 196801 (2011)
[3] Kentaro Nomura1 and Naoto Nagaosa, PRL 106, 166802 (2011)
[4] Kantser, V. G, Lelyakov, I. A. Malkova, N. M., Semiconductors vol. 26, p. 896-899, (1992)
[5] Kantser V., Malkova N, PhysRevB.56,p.2004, (1997)
[6] H. D. Li, Z. Y. Wang, X. Guo, T. L. Wong, N. Wang, and M. H. Xie, Appl Phys Lett 98 (4) (2011)
[7] B. A. Bernevig, T. L. Hughes, and S. C. Zhang, Science, vol. 314, pp. 1757, 2006.
[8] I.Begenari,V.Kantser NanoLett, in press
[9] P. Ghaemi, Roger S. K. Mong and J. E. Moore, cond-mat 1002.1341v2, (2010)