Topological Interface States and Effects for Next Generation of Innovative Devices

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***Abstract* — Topological insulators (TI) have opened a gateway to search new quantum electronic phase of the condensed matter as well as to pave new platform of modern technology. This stems mainly on their unique surface states that are protected by time-reversal symmetry, show the Dirac cones connecting the inverted conduction and valence bands and exhibit unique spin-momentum locking property. Increasing the surface state contribution in proportion to the bulk of material is critical to investigate the surface states and for future innovative device applications. The way to achieve this is to configure topological insulators into nanostructures, which at the same time in combination with others materials significantly enlarge the variety of new states and phenomena. This article reviews the recent progress made in topological insulator nanoheterostructures electronic states investigation. The state of art of different new scenario of engineering topologicaly interface states in the TI heterostructures are revealed, in particular by using polarization fields and antiferromagnetic ordering. Some of new proposals for innovative electronic devices are discussed.**

***Index Terms* — Topological insulator,heterostructures, nanowire, nanotube, Dirac cone, supersymmetric potential, polarization fields, antiferromagnetic ordering, low dimensional thermoelectricity.**

I. INTRODUCTION

Topological insulators (TI) represent a new class of materials and they have sparked a massive search for new states and phenomena in condensed matter physics.
A TI can easily be identified by a few simple rules: the presence of large spin–orbit coupling, an odd number of band inversions between the conduction and the valence band by increasing the average nuclear charge, and a sign change of the symmetry of the molecular orbitals.

Part of interest in TIs stems from the fact that they represent a new topological phase of noninteracting electrons: the TI character of a material is its bulk property, nontrivially encoded in the wavefunctions of the occupied (valence band) states. However, it is the presenceof the helical edge/surface states which leads to observable consequences. Their surface states are protected by time-reversal symmetry and show the Dirac cones connecting the inverted conduction and valence bands [1]. 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.. These Dirac cones constitute the topological transport regime, which has the gapless conducting and spin-momentum locked surface states leading to the suppression of backscattering. Such extraordinary surface states of the three-dimensional topological insulators may occur, as the term ''surface'' already suggests, only at the surfaces or, more generally, interfaces where the topological invariant changes [2].

Unlike graphene, the states on the Dirac cone on the surface of the TI are spin filtered; they have fixed spin directions for each wave number k. In such way among many new topics developed in such materials and nanostructures, the most exciting one may be spintronics. Spintronics (or spin-electronics) is the term to express a field of electronics utilizing both charge and spin degrees of freedom possessed by an electron, which have been treated independently until recently.

Because the state at k and that at –k have the opposite spins, the perfect backscattering from k to −k is forbidden. The gapless helical surface states with linear dispersion is similar to photons.Therefore, when two different TIs are attached together, the refraction phenomenon similar to optics is expected at the junction.

Exploring the properties of nanoscale topological insulators is a growing area of research and the present paper reveals some aspects of new interface and device physics of such materials. the spectrum and characteristics of topological interfaceface states (TIS) 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 main part of the paper. 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 ELECTRONIC STATES OF TI HETEROSTRUCTURES

We consider a junctions at z = 0 between between TI and BI or (another TI) The electronic states of such materials are described by the same type of low-energy effective 3D Hamiltonian [3], which has the 4 × 4 matrix form and can be expressed in general form as

$$H=\begin{pmatrix} \Delta(z)+V(z) & \vec{\sigma}\,\vec{p}-i(\vec{\sigma}\,\vec{u}+L) \\ \vec{\sigma}\,\vec{p}+i(\vec{\sigma}\,\vec{u}+L) & -\Delta(z)+V(z) \end{pmatrix} (1),$$

where σ are the Pauli matrices, $\Delta=E_g/2+M1k^2_z+M2k^2$, $\vec{p}=-i\hbar\left(v_\perp\nabla_x, v_\perp\nabla_y, v_{||}\nabla_z\right)$, $v_{||}$, $v_\perp$ are the electron Fermi velocities, and V(z) is the potential, which incorporates the change in the work function in the structure and applied gate voltage.Following the results of our early works [4] we introduced the vector parameters u which describes the electrical polarization and the scalar L to describe the antiferromagnetic ordering with the antiferromagnetic vector along z-axis.

The junction breaks translation symmetry in the z-direction, and we let kz → −i∂/∂z to obtain a system of second order homogeneous differential equations H(k→ −i∂/∂z)χ = Eχ. They are solved with the ansatz of the effective mass approximation.

We firrst analyze topological states bound to the inteface of TI and BI like PbTe/SnTe without antiferromagnetic ordering *L=0* and electrical polarization *u=0*. In this case the energies of the TIS are

$E=E_0\pm\frac{v_\perp k_\perp D}{\Delta_1-\Delta_2}$, where

$D^2=(\Delta_1-\Delta_2)^2-(V_1-V_2)^2$ and

$E_0=(\Delta_1V_2-\Delta_2V_1)(\Delta_1-\Delta_2)^{-1}$.

In Fig. 1 we show TIS energy dispersion of the [111] valley states formed at the PbTe/$Pb_{1-x}Sn_xTe$ heterointerface in the configuration of wide quantum well.

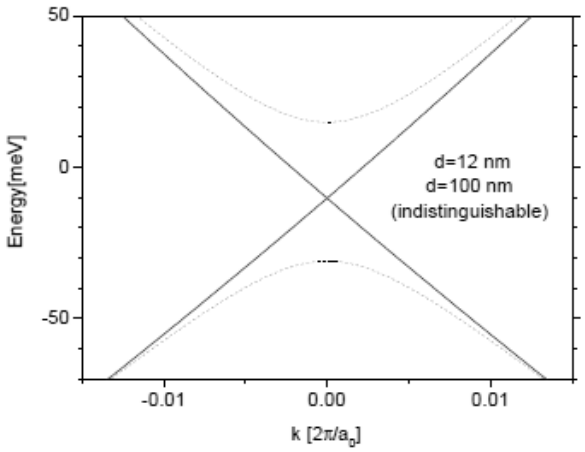

Fig. 1. Energy dispersion of TIS for $PbTe/Pb_{0:54}Sn_{0:46}Te$ quantum well grown in [111] direction, with PbTe widths d of 12 and 100 nm (undistinguishable), plotted as a function of inplane wave k vector.

The helical nature of these states can be seen by calculating the expectation values of spin operators , i.e. the spin vector is perpendicular to k, pointing clockwise (anticlockwise) for negative (positive) energy branch.

This helical nature of surface topological states of TI leads to new interface physics of heterojunction of two TI. In the case of two TIs, at the junction we expect a coupling between two surface states belonging to different TIs. In the framework of a simple model [5] which includes phenomenological coupling between massless relativistic states of the two TIs, it was shown earlier that the properties of the junction surface states strongly depend on the relative sign of the Fermi velocities of the two Tis. The analysis was performed on the basis of the refraction phenomena on the junction between the two TI surfaces with different velocities. The resulting reflectance and transmittance reflect the backscattering-free nature of the surface states of TIs. When the velocities of the TI surface states for the two TIs have different signs, we show that the gapless states appear on the interface (Fig.2). The existence of the gapless states is shown by using the mirror Chern number, and thus is topologically protected by the mirror symmetry.

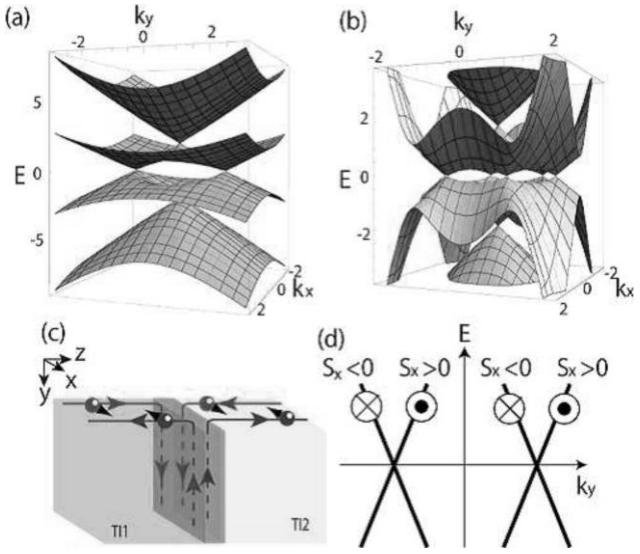

Fig.2. Dispersion on the TIS between the two TIs in Eq. (5) with different velocities

Another investigations [6] shows that the junction surface states of two TIs, in certain situations, can exhibit superluminal (tachyonic) dispersion of Dirac fermions. The obtained results indicate that for general variation of the parameters of TI-2, the junction surface states show one branch with unique dispersion relation that resembles the dispersion of the tachyons. The existence of a tachyonic branch in the dispersion relation of junction states means that the energy dispersion becomes a non-analytic function of the 2D surface momentum, i.e., the group velocity $v_g=\hbar^{-1}\partial E(k)/\partial k$ is infinitely large.

A systematic study of the possible combinations of Tis was performed in [7] using a quantitative model for a strong TI and the existence of different types of topological interface states was demonstrated (Fig.3). These interface states are not protected in the same manner as the surface states of a single TI, instead they are protected by mirror symmetry. The physics of this system resembles certain aspects of bilayer graphene, because both result from the hybridization of Dirac cones.

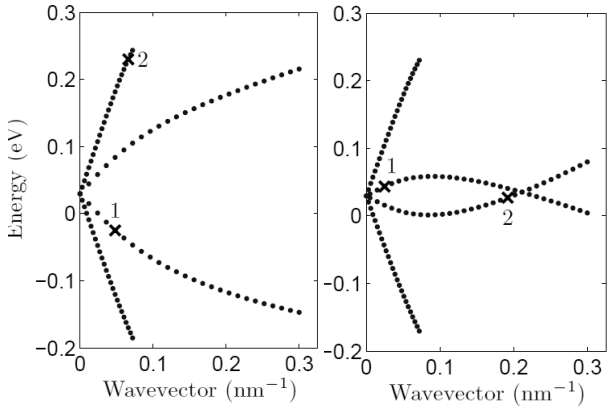

Fig.3. Dispersion of the TIS between TIs for the cases: i)when the velocities in the junction are opposite sign,but in the perpendicular direction – the same; ii) wheh both velocities change the sign across the junctin.

III. TOPOLOGICAL ELECTRONIC STATES OF TI HETEROSTRUCTURES INDUCED BY ELECTRICAL POLARIZATION AND ANTIFERROMAGNETIC ORDERING

Further we analyse on the basis of the Hamiltonian (1) the TIS for topological insulator heterostructures with incorporated electrical polarization *u* using the metod of supersymmetric quantum mechanics. We assume that the spatial variation of the quantities Δ, u and V is determined by the same function $f(z)$: $\Delta(z)=\Delta_+ -\Delta_- f(z)$, $u(z)=u_+ -u_- f(z)$, $V(z)=V_0 f(z)$, where $\Delta_\pm=(E_{gb}\pm E_{ga})/4$, $u_\pm=(u_{gb}\pm u_{ga})/2$, and $f(z\to\pm\infty)=\pm 1$.

To study the energy spectrum of a nonuniform structure consisting of a heterojunction, we transform eq 1 into an equation of supersymmetric quantum mechanics [4]

$$\left\{\begin{array}{l}\left[p_x^2+W^2(z)+\hbar v_{II}\sigma_z\otimes\tau_x\dfrac{dW(z)}{dz}\right]\\ +\Delta_+^2+(\pm p_\perp+u_+)\\ -E^2\dfrac{\left[\Delta_+\Delta_-+\Delta_-(\pm p_\perp+u_+)+EV_0\right]^2}{\Delta_-^2+u_-^2-V_0^2}\end{array}\right\}\Phi(z)=0, \quad (2)$$

where W(z) is the supersymmetric potential and is given by $W(z)=(\Delta_-^2+u_-^2-V_0^2)^{1/2}$

$$\left[f(z)+\frac{\Delta_+\Delta_-+u_-(\pm p_\perp+u_+)+EV_0}{\Delta_-^2+u_-^2-V_0^2}\right]$$

According to a theorem of supersymmetric quantum mechanics [4], when the asymptotic expression for the superpotential $W(z\to\pm\infty)$ have opposite signs, i.e. when $\left|\dfrac{\Delta_+\Delta_-+u_-(\pm p_\perp+u_+)+EV_0}{\Delta_-^2+u_-^2-V_0^2}\right|\le 1$, Eq 2 has so-called zero mode as eigenvalue. The energy spectrum of the TIS is not degenerate in terms of spin and it is determined from

$$E=\left\{\begin{array}{l}-\Delta_+(V_0\Sigma_-+Du_-)+\\ (\pm p_\perp+u_+)(D\Delta_-+V_0u_-)\end{array}\right\}(\Delta_-^2+u_-^2)^{-1}, \quad (3)$$

for $(V_0D-\Delta_-u_-)(u_-^2-V_0^2)^{-1}\ge 0$, where $D=(\Delta_-^2+u_-^2-V_0^2)^{1/2}$ and $V_0\le(\Delta_-^2+u_-^2)^{1/2}$.

This solution determines two-dimensional boundary electronic states of the TIS type, which are localized near the interface.TIS exist in limited intervals of the energy and the transverse momentum $p_\perp=\hbar v_\perp k_\perp$. These intervals are defined by

$$V_0+\frac{\Delta_++\Delta_-}{u_-^2-V_0^2}(u_-D-V_0\Delta_-)\le E \le -V_0-\frac{\Delta_+-\Delta_-}{u_-^2-V_0^2}(u_-D+V_0\Delta_-), \quad (4)$$

$$u_--\frac{\Delta_+-\Delta_-}{u_-^2-V_0^2}(u_-\Delta_--V_0D)\le u_+\pm p_\perp \le -u_--\frac{\Delta_++\Delta_-}{u_-^2-V_0^2}(u_-\Delta_-+V_0D) \quad (5)$$

We easily see from (4) and (5) that TIS arise only if $\Delta_-u_-\le 0$. Consequantly, if $\Delta_-u_->0$, two-dimensional electronic states appear at the heterojunction only at finite values of the difference between work functions $V_0\ne 0$. In this case TIS bands lie against the background of either bulk conduction bands.

The proposed TI heterostructures driven by electrical polarization has many unique advantages, including: 1) it can be realized based on commonly used semiconductors and be integrated into various devices; 2) itis driven by large intrinsic polarization fields; 3) the TI state can be manipulated by applying external fields or injecting charge carriers and can be adjusted by standard semiconductor techniques, including doping, alloying and varying the QW thickness; 4) The proposed TI has many unique advantages, including: 1) it can be realized based on commonly used semiconductors and be integrated into various devices; 2) it is driven by large intrinsic polarization fields; 3) the TI state can be manipulated by applying external fields or injecting charge carriers and can be adjusted by standard semiconductor techniques, including doping, alloying and varying the QW thickness; 4) the polarization field can induce a large Rashba SOI in this system containing only light elements, which provides a new approach to manip- ulating spin freedom in such systems.caninduce a large Rashba SOI in this system containing only light elements, which provides a new approach to manipulating spin freedom in such systems.

To ilustrate the generation of TI states driven by the polarization field recently [8] the edge states of a Hall bar of GaN/InN/GaN quantum well have been analysed (Fig.4). The kp simulations show that the band structure of the GaN/InN/GaN QW is inverted when the QW width is larger than 1,55 nm. The presence of edge states in the gap between E1 and LH1 subbands is clearly demonstrated, and the distribution of these states in real

space shows that they are highly localized in the vicinity of the edges of the Hall bar. These edge states are topologically invariant under scattering, and therefore the corresponding mean free paths of the carriers can be exceedingly large.

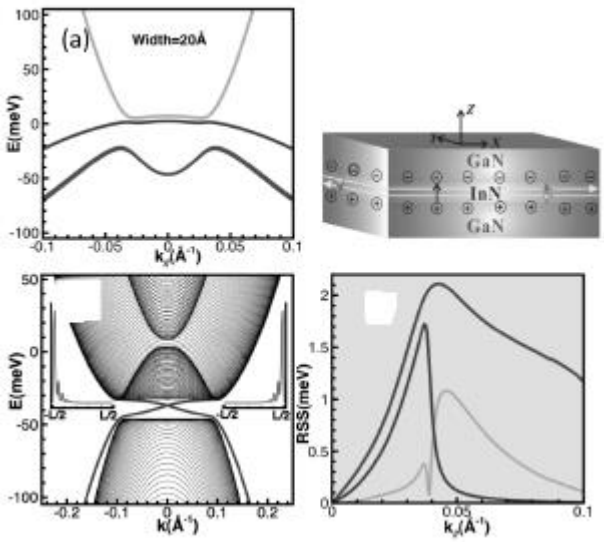

Fig.4 Band structure of a GaN/InN/GaN QW obtained on the basis of band kp model.

Another opportunity to tailor the TIS is offered by the antiferromagnetic ordering of the materials, which constituted heterostructure. In the simplest form this situation is described by Hamiltonian (1). After the transformation

$U = \begin{pmatrix} i\sigma_z & 0 \\ 0 & 1 \end{pmatrix}$, the Hamiltonian (1) become

$$H = \begin{pmatrix} \Delta(z) & ip_z + W + u \\ -ip_z + W + u & -\Delta(z) \end{pmatrix}, \qquad (6)$$

where $W = \vec{\sigma}[p\vec{u}] + \sigma_z L$.

The energy spectrum of bulk materials consists of the four spin-split energy branches (Fig.5)

$$E_{1,2}^{+} = \left((u + W_{\pm})^2 + \Delta^2 + p_z^2\right)^{1/2} \qquad (7)$$

$$E_{1,2}^{-} = -\left((u + W_{\pm})^2 + \Delta^2 + p_z^2\right)^{1/2},$$

where $W_{\pm} = \pm\left(L^2 + p_{\perp}^2\right)^{1/2}$.

Using the anzatz of the supersymmetric quantum mechanics with the same spatial variation of the quantities Δ , u ,Land V determined by the same function $f(z)$ we obtaine the following solution of the TIS

$$E = \mp\left\{\left(u_0 V_0 - \Delta_0\left(u_0^2 + \Delta_0^2 - V_0^2\right)^{1/2}\right)\left(\Delta_0^2 + u_0^2\right)^{-1}\right\} \times \left(p_{\perp}^2 + L^2\right)^{1/2}, \qquad (8)$$

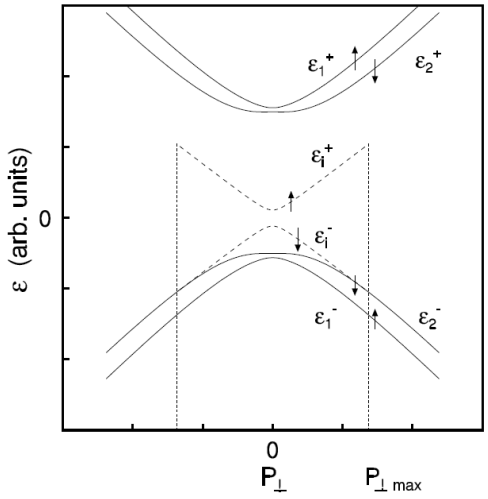

Fig.5 Energy spectrum of topological interface states in the heterostructure with antiferromagnetic ordering and electrical polarization.

The obtained states are of the inteface type because its wave function is localized at the interface boundary.Taking into account the supersymmetric we obtaine the range of TIS existence,which is determined by

$$(p_{\perp}^2 + L^2)^{1/2} \le \begin{bmatrix} (\Delta_0^2 + u_0^2)(u_0^2 + \Delta_0^2 - V_0^2)^{1/2} \\ \times (\Delta_0 V_0 + u_0 (u_0^2 + \Delta_0^2 - V_0^2)^{1/2})^{-1} \end{bmatrix}$$

Comparing the expression (7) for the energy levels of the homogeneous semiconductors and (8) for interface heterojunction states one gets that the interface states are situated nearer to the middle of the gap of the constituents (Fig.5). Thus if in the studied semiconductor heterojunctions the Fermi level, for example by means of doping, gets into one of the two-dimensional interface bands, then it leads to the magnetic ordering into the interfaceplane. The magnetic moment as it follows from the analysis is exponential attenuated moving away from the interface plane.

IV. TUNABLE TOPOLOGICAL STATES IN NANOWIRES AND NANOTUBES

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 topological surface state.

In this part of the paper the TIS of cylindrical nanowires and topological insulator Bi2Te3 with cylindrical pores are analysed. The developed low-energy Hamiltonian (1) for bulk Bi2Te3 is adequate to highlight TIS on the cylindrical surface.

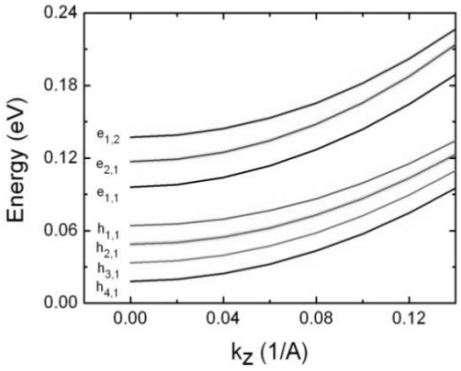

Fig.6. Electronic structure of TI Bi2Te3 nanowire with a radius of 10 nm.

The TIS forming inside the bulk gap (Fig.6) 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 TIS modes of cylindrical surface have a finite gap described qualitatively by relations Egs ~v/R (Fig.6). In results nanowire and nanopore composites of TI have distinct pecularities from layered ones and offer new opportunities in tailoring the properties of nanostructures.

Figure 7 depicts a dependence of the direct band gap at the Γ point of the TI Bie2Te3 and Bi2Se3 nanowires on radius. The band gap depends nonmonotonically on radius. It achieves a minimum value of 0.012 (0.03) eV at a Bi2Te3 (Bi2Se3) NW radius of 30 nm. Therefore, by adjusting NW radius, the band gap can be decreased by 50 (15) times compared to the corresponding value of 0.6 (0.56) eV at the Γ point for the Bi2Te3 (Bi2Se3) bulk material.

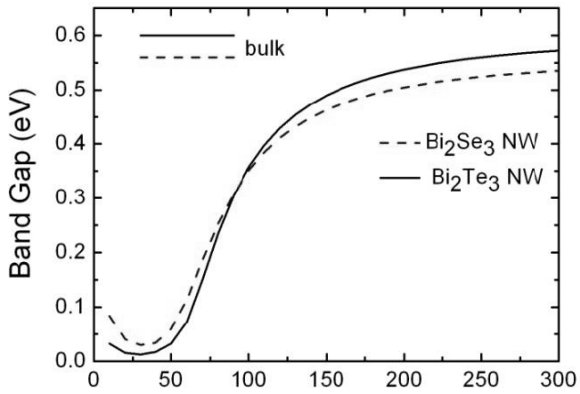

Fig.7 Dependence of the direct band gap at the Γ point of the topological insulator Bie2Te3 (solid line) and Bi2Se3 (dashed line) nanowires on radius.

Figure 8 describes the electronic structure of the TI Bi2Te3 nanotube with an external radius of 60 nm and internal radius of 10 nm. Here, the first 3 (4) electron (hole) modes e1,1, e2,1, and e3,1 (h1,1, h2,1, h3,1, and h4,1), corresponding to different values of angular momentum quantum number and radial quantum number being equal to 1, are presented.

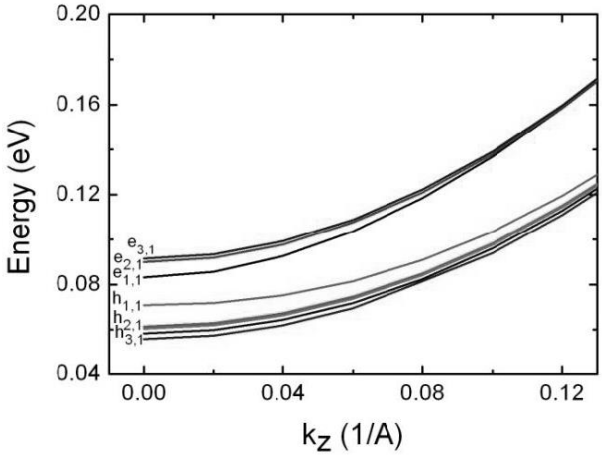

Fig.8. Electronic structure of TIS Bi2Te3 nanotube with an external radius of 60 nm and internal radius of 10 nm. The origin is at the Γ point.

The origin of the graph is set at the Γ point. The Bi2Te3 material is an indirect band gap semiconductor, as a result, both electron and hole energy dispersion curves increase with wave vector at the vicinity of the Γ point. A splitting between the hole subbands and their dependence on ratio b/a is much greater compared to that for electrons, because the effective hole mass is less than the electron effective mass. With increasing of wave vector, the electron (hole) modes merge. The electron and hole ground states (e1,1 and h1,1) are located near the bottom of the conduction band of the bulk material and they are located away from other subbands.

V. TOPOLOGICAL INSULATOR NANOSTRUCTURES AND ENHANCED THERMOELECTRICAL PERFORMANCE

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,nanotube and nanowire of Bi2Te3. To estimate the surface contribution of TI to the transport coeffcients we assume the bands to be Dirac-like with a subgap and use Boltzmann equation in the relaxation time approximation [9].We show that by making holes in these TI materials and inducing subgap in their surface states by means of geometrica land others factors one can significantly enhance their thermoelectric eficiency.The high density of holes in the direction of transport has two positive effects: 1) to trap
phonons and thus reduce the thermal conductivity; 2) to increase the surface to bulk ratioand therefore effectively enhance the electric conductivity of the sample. The effect of the

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 9).

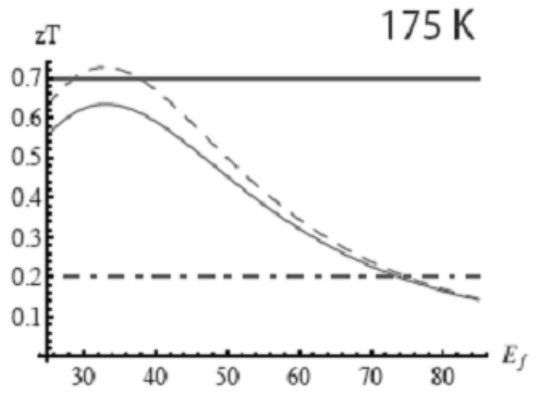

Fig .9. ZT for the thin film including bulk contributions at 175 Kelvin. The straight line in each figure corresponds to the best known ZT at the same temperature. Dashed line indicates the ZT for the surface states alone and Dashed-Dotted line indicates ZT for bulk Bi2Te3.

As is evident from Fig. 9, 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 Bi2Te3 thin films. The same approach applies as well to nanowires.

CONCLUSIONS

Due to their unique ability to form new electronic phase and generate new phase of the electronic systems at the surface and interface topological insulators stem at present in the center of materials and device physics investigations. Unique peculiarities of the topological surface states related to time-reversal symmetry, Dirac cones attributes of the spectrum and spin-momentum locking property open new gateway to reconfigure the electron systems at the contact of TI with BI as well as at the junction of two different TI. TSS in heterojunctions are converted in new type of two-dimensional electronic states – TIS - with very reach physics and new useful attributes to design electronic devices. A systematic study of the possible combinations of TI heterojunctions was performed and the existence of different types of topological interface states was demonstrated. Polarization fields and antiferromagnetic ordering was shown to be the drivers of new type of TIS. Due to spin-momentum locking property the evolution of TSSin nanowires and nanotubes has new qualitative attributes. A one-dimensional (1D) electron waveguide with modes indexed by the half-integer total angular momentum j is formed, where each mode contains a right and a left-mover. The spin direction is always tangential to the surface and perpendicular to the momentum. The gap in nanowires and aother nanostructures can be opened and in the results increased thermoelectric performance can occur as well as new ways of electronic dedevices.

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