Posters
(in alphabetical order, part 2)

P16

Fabrication of pure α-Sn films

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Ways of fabricating strained α-Sn film on InSb substrate were established long before this particular material was theoretically predicted to be elemental 3D topological insulator. However, further investigation of its topological surface states and topological charge carriers made much higher demands regarding the surface quality of this material. It is known that the purity of the α-Sn surface is disrupted if substrate is heated during film growth, which induces strong In diffusion to the top layers, changing the electrical properties of the film. Also, use of dopants prior (Bi) and during (Te) α-Sn growth to improve surface quality raises many questions about the surface morphology and the origin of the possible surface states. We have developed a modified fabrication process of α-Sn films on InSb (100) without heating of the substrate during growth nor use of any dopants. Crucial modification was made in the substrate preparation process which includes Ar^+ ion-beam etching using two energy modes (500 and 1000 eV) and different stages of annealing. After the substrate preparation Sn film was grown by Molecular Beam Epitaxy in the UHV condition on the temperature around 285 K. Multiple techniques were employed to confirm achieved chemical purity and structural properties of the film and this data will be presented fully. A closer look into the surface morphology of α-Sn films is done by Scanning Tunneling Microscopy (STM).

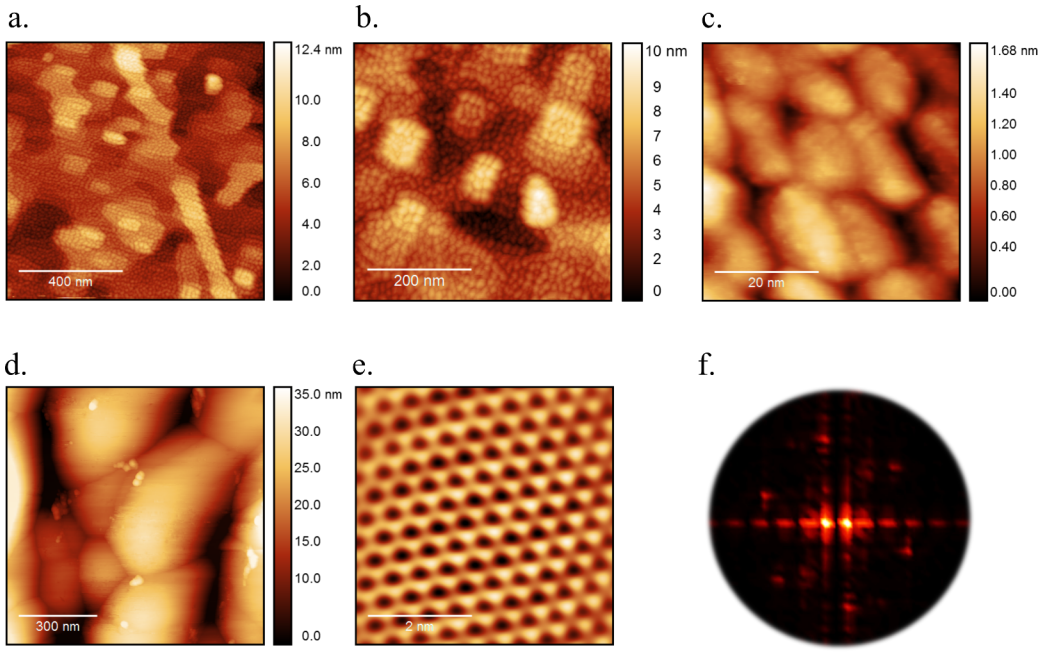

Figure 1: STM images of the α-Sn films
a. b. and c. STM images of Sn sample grown on 285 K,
d. STM image of Sn sample grow on 330 K,
e. FFT filtered STM image of atomic resolution (buckling honeycomb),
f. FFT pattern of the atomic resolution STM image.

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Terahertz emission study of Sb_2Te_3 and Bi_2Te_3 films

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Telluride-based three-dimensional topological insulators (TIs) are promising for new optical and electrical applications as they have topological surface states (SS) as well as phase change property and high thermoelectric performance. To understand the topological nature and electrical properties, terahertz (THz) spectroscopic techniques are powerful experimental tools since the energy of THz radiation is much smaller than the bulk band gap energy of TIs. Indeed, we reported significant difference in the THz properties between Ge-Sb-Te phase change alloy material and GeTe/Sb_2Te_3 multi-layered system, where GeTe is a normal insulator and Sb_2Te_3 is a TI. [1]

In this study, we observed photo-induced THz radiation from thin films of Sb_2Te_3, Bi_2Te_3, and their heterostructure (Bi_2Te_3/Sb_2Te_3). Sb_2Te_3 is a *p*-type TI and Bi_2Te_3 is a *n*-type TI which has a second SS located ∼1.5 eV above the first SS. [2] A Ti:Sapphire femtosecond laser (800 nm) was employed to excite the samples and detect emitted THz fields. The samples were irradiated with a femotosecond pulse and the emitted THz field was measured by a dipole antenna.

Figure 1 shows typical time-domain signals of *p*-polarized THz radiation from the samples. From all samples, clear transient signals of THz radiation were observed. It was found that the direction of the *p*-polarized THz field from Sb_2Te_3 is opposite to that from Bi_2Te_3. Based on the polarization dependence of the emitted THz radiation, we attributed the generation process of *p*-polarized THz radiation mainly to transiently accelerated carriers parallel to the sample normal direction. The difference in the polarity of *p*-polarized THz fields observed for Sb_2Te_3 and Bi_2Te_3 implies that the photo-induced instantaneous modification of the depletion field on the sample surfaces is the dominant mechanism of THz emission. [3] The shape of the *p*-polarized THz field for the Bi_2Te_3/Sb_2Te_3 sample is different form others and hence is thought to be related to the interface state.

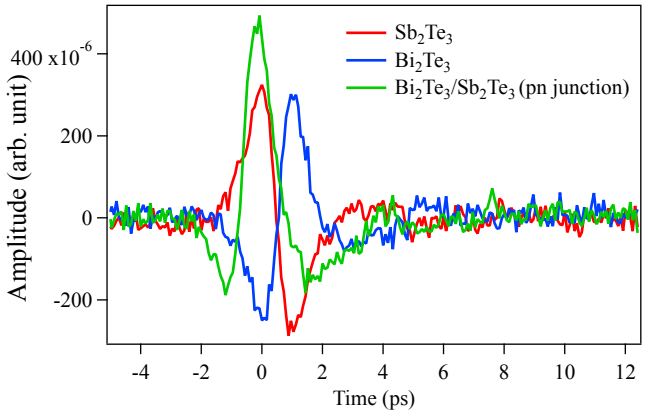

FIG. 1. Transient *p*-polarized THz emission signals for Sb_2Te_3, Bi_2Te_3, and Bi_2Te_3/Sb_2Te_3 films.

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P18

Spin polarization of Dirac-cone surface state at W(110) influenced by polarized light

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Recently, for the topological surface state (TSS) of Bi_2Se_3, several groups have observed an interesting phenomenon by spin- and angle-resolved photoemission (SARPE): the observed spin features of the photoelectrons are strongly dependent on the light polarization [1,2]. This effect is currently highly debated in the field of optospintronics. Although this effect might be dependent on crystal symmetry, so far, the observations of the effect are limited to surfaces with C_{3v} symmetry[1-3]. Very recently, we have discovered that the surface of W(110) shows a spin-polarized Dirac-cone state within a spin-orbit-induced gap, which is reminiscent of a TSS [4]. Here, in contrast to so-far studied topological insulators, the surface structure has C_{2v} symmetry. The C_{2v} symmetry strongly influences the dispersion of the Dirac-cone surface state, resulting in a flattened Dirac-cone. W(110) is suitable to research the spin feature of the photoelectrons dependent on the light polarization on material with C_{2v}.

We have studied the spin feature of Dirac-cone surface state along , at W(110), using SARPE spectroscopy with various light polarizations; left and right circular or *s*- and *p*- polarizations. We have noted that the observed spin feature of photoelectrons excited by *p*-polarized light is opposite to the case of *s*-polarized light for tangential spin component. According to dipole selection rule, we can observe the spin feature of even orbital symmetry and odd orbital symmetry by *p*-polarized light and *s*-polarized light, respectively. In that, their results show the orbital dependence of spin feature of the Dirac-cone-like surface state [5].

On the other hand, in the case of circular polarized light, not only tangential spin component but also radial and out-of-plane spin component can be observed. The observed complex spin feature accepts strongly influenced by C_{2v} symmetry and is well reproduced by first-principles calculation including photoemission process. In detail, I introduce you in my presentation.

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P19

Time Resolved Spectroscopy in a Narrow Gap Semiconductor with Surface InAs Two-dimensional Electron System

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Compound semiconductors such as InAs and InSb have unique properties including small effective masses, high electron mobilities, and large g-factors[1–5]. This makes these materials suitable for a variety of device applications including: Mid-Infrared Quantum Cascade Lasers[6], Geometrical Magneto-Resistance[7], in addition to 'hot-carrier' solar cells, where the phonons can live long enough to be absorbed by the excited carrier. Epitaxial two-dimensional heterostructures containing InAs layers are also considered to be suitable for spintronics[1], topological, and superconducting quantum computation applications[8,9]. Here we present the carrier dynamics of these heterostructures, important for developing optoelectronic devices. These measurements will allow us to understand several scattering processes such as carrier-carrier and carrier-phonon[5]. In this study we employed a degenerate pump/probe scheme, where the source was a Ti-sapphire laser with near infrared (NIR) pulses with duration of 100 fs and a repetition rate of 80 MHz. In this scheme, as shown in Fig. 1 for one of the measurements, the pump/probe were tuned at 700 nm, where we excited and probed within $\sim$ 220 nm thickness of this heterostructure. The photo-excited carriers show a long relaxation lifetime and our systematic time resolved measurements will provide important information, for variety of applications, in a high mobility narrow gap system with a 2DEG at the surface.

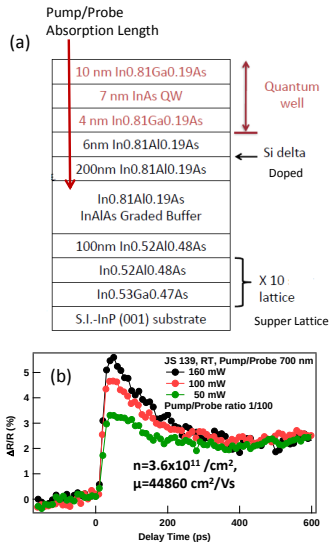

FIG. 1: (a) Layer structure of high mobility epitaxial two-dimensional heterostructure. (b) Differential reflectivity as a function time for pump/probe tuned at 700 nm at different pump powers.

0.1. Acknowledgment:

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P20

THz magneto photoresponse spectroscopy of structurally asymmetric $InAs/Al_{0.2}Ga_{0.8}Sb$ QW

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InAs/GaSb semiconductor heterostructure were known as a prototype of broken gap type-II quantum well (semimetalic) system for a while. Recently, it turns out that such heterostructures could host novel quantum state of materials known as topological insulators (2D case) due to its band inversion [1,2]. We studied band structure configuration of $InAs/Al_{0.2}Ga_{0.8}Sb$ heterostructure with broken gap (type II) band alignment through solving 8×8 Kane model Hamiltonian using vurgaftmans parameters. Due to Aluminum content of QW (InAs) barrier layers we observe a smaller overlapping between conduction and valence band at barrier regions. Furthermore, we investigated magneto-transport and THz magneto photoresponse [3] properties of Hall bar samples made of MBE grown wafer with same heterostructure configuration. The carrier density of QW region turns to be $n_s=7.6\times10^{11}$ cm^{-2} obtained from quantum oscillation frequency (SdH ferq.) of Rxx signal at T=1.7 K. this carrier density is such that sample has semimetalic phase with hall mobility of $\mu = 2.5\times10^5$ $cm^{-2}/V\cdot s$. Results from two band model also confirms the broken band alignment of our sample with phase transition at x=0.26 of alloying composition for barrier layers with 10 nm thick InAs QW. The sample also exposed to chopped THz wave at f=2.53 THz to get PR signal which have been used to extract different physical parameters of 2DEGs. Investigating charge carrier properties of such novel heterostrcurure configurations could pave the way for fabricating practical devices (e.g. transistors, IR lasers) benefiting properties of quantum materials. We plan to present our findings for $InAs/Al_{0.2}Ga_{0.8}Sb$ heterostructure system at NGS18 conference.

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P21

Topological invariants for disordered systems

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We present an algorithm to obtain real space markers of topological invariants, that do not rely on the periodicity of the system, and we use them to study disordered systems in various topological classes. In this algorithm, we boost the efficiency of the topological markers by using the most localized approximation of the band projector.

The band projector is expanded with the kernel polynomial method (KPM) [1] and it is the most localized approximation, at a given energy resolution, for general hamiltonians. The efficiency of our algorithm relies on the locality of the projector operator and its KPM expansion, where each moment of the expansion is obtained recursively, applying the Hamiltonian to a local vector. Each order of the expansion *spreads* the local vector in real space, and, at the same time, increases the precission of the approximation in energy. Therefore, setting an energy resolution of the expansion, also sets the minimum size of the sample, in order to mimic an infinite system.

We apply this systematic approach for the cases of 2D Chern makers [2] and 3D topological invariants in classes BDI and AIII [3, 4]. The algorithm can be further extended to other noncommutative expressions [5] for other topological classes, making it a powerful tool to study the effect of disorder on the topology of large scale systems.

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P22

A Study of Bi-Te Stoichiometric Family: Switching from Strong to Weak Topological Phase & Beyond

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Topological Insulator is relatively a new class of materials in condensed matter physics. Strong spin-orbit coupling in such materials leads to band inversion which results in linearly dispersed spin polarized energy states. Outcome of this phenomenon is appearance of metallic (edge in case of 2D and surface in case of 3D) states with insulating bulk band structure being protected by time reversal symmetry (TRS). 3D Topological Insulators are classified into two categories i.e. strong topological insulators (STI), where all surfaces exhibit metallic behavior and topology is protected by TRS; and weak topological insulators (WTI) where topology is exhibited only by specific surfaces.

In this study we have focused on optimizing the growth of high quality thin film using Molecular Beam Epitaxy (MBE), crystal structural analysis using X-Ray Diffraction (XRD) and Scanning Transmission Electron Microscopy (STEM) and electronic structure investigation using Angular-Resolved Photo Emission Spectroscopy (ARPES) of Bi-Te stoichiometric compounds. Bi_2Te_3 is the most commonly known and heavily studied member of this family. It contains the highest contents of Te and grows in the form of Quintuple Layers (QL) with weak Van-der-Waals gaps. Bi_2Te_3 is a STI with all metallic surfaces protected by TRS. Detailed structural analysis and electronic investigations are performed [1]. With controlled reduction of Te contents high quality thin films of Bi_1Te_1 are obtained [2]. Bi_1Te_1 is comprised of natural superlattice of alternating two Bi_2Te_3 QLs and one Bi bilayer. It is found to exhibit the WTI behavior with non-protected trivial surfaces normal to the layer stacking orientation. Along with WTI, it also exhibits partially polarized surface states away from the Γ point which confirm the Topological Crystalline Insulator (TCI) phenomenon where topology is not anymore protected by TRS rather by Crystal Symmetry (CS). Hence, Bi_1Te_1 is a dual topological Insulator exhibiting WTI and TCI characteristics simultaneously [2]. GW calculations are found to be in agreement with results obtained via ARPES. With further controlled reduction of Te contents Bi_4Te_3 films have successfully been grown and are subject to future investigations.

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P23

Towards Microscopic Control of the Magnetic Exchange Coupling at the Surface of a Topological Insulator

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Magnetically doped topological insulators may produce novel states of electronic matter, where for instance the quantum anomalous Hall effect state can be realized. Pivotal to this goal is a microscopic control over the magnetic state, defined by the local electronic structure of the dopants and their interactions. We report on a systematic study of the distance dependent magnetic coupling among Mn or Co atoms adsorbed on the surface of the prototypical topological insulator Bi_2Te_3.

We compare our ab-initio calculations with x-ray magnetic circular dichroism measurements, which allows us to uncover the mechanisms of the exchange interaction between magnetic atoms coupled to the topological surface state in strong topological insulators. We find that the sign of the magnetic coupling at short adatom-adatom distances is opposite for Mn with respect to Co. For both elements, the magnetic exchange reverses its sign at a critical distance between magnetic adatoms, as a result of the interplay between superexchange, double exchange and Ruderman-Kittel-Kasuya-Yosida interactions.

The detailed understanding of the underlying mechanisms opens the possibility for a fine tuning of the magnetic interactions and demonstrates that surface-doped topological insulators pose an ideal platform to investigate the emerging physics on the brink of topology and magnetism.

We acknowledge financial support from the DFG (SPP-1666) and from the VITI project of the Helmholtz Association as well as computational support from the JARA-HPC Supercomputing Centre at the RWTH Aachen University.

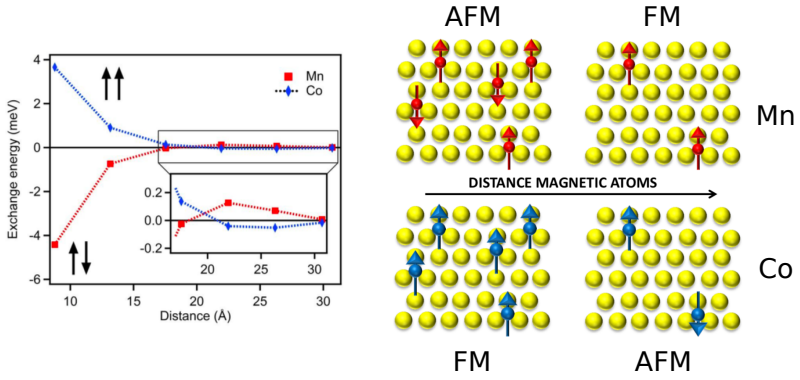

Figure 1: Distance dependence of the magnetic exchange coupling strength of Mn and Co doped Bi_2Te_3. As a consequence of the interplay of short-distance exchange mechanism and long-distance RKKY exchange interactions the favored magnetic ordering of the magnetic atoms on the surface can be finely tuned.

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Surface effects in topological insulators A_3Bi (A alkali element)

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Surface electronic spectra, surface and bulk properties as well as the underlying chemical bonding characteristics are considered on the example of polar intermetallics KNa_2Bi, K_3Bi and Rb_3Bi [1, 2]. Chemical bonding in this materials have been analized within the Bader charge population analysis, and the MLWF technique. We pinpoint the emergent surface features in the electronic spectra that are driven by the chemical bonding. Our findings build up a fundament for a more generalized, realistic study of polar intermetallics A_3Bi within a model method and, hence, promote better understanding of other topologically distinct systems with similar chemical bonding characteristics.

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P25

The Anomalous Hall Effect in Magnetic Topological Insulators

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We have studied the anomalous Hall effect (AHE) on the surface of a 3D magnetic topological insulator, which provides a deep insight into the interplay between magnetism and the transverse transport of massive Dirac Fermions due to an external applied electric field. In this work, the AHE in a 3D TI is investigated using the semi-classical Boltzmann approach along with a modified relaxation time scheme, in terms of the chemical potential of the system, the spatial orientation of the surface magnetization and the concentration of magnetic and non-magnetic impurities. All three different contributions to the AHE -the intrinsic berry-phase curvature effect, the extrinsic side-jump and the skew scattering effects- are systematically treated. By applying a fully analytical method we show how the relative importance of these contributions can be tuned, and can even turn-off the AHE. For example it is shown that the anomalous Hall conductivity can even change sign by altering the orientation of the surface magnetization, the concentration of the impurities and also the position of the chemical potential, in agreement with recent experimental observations.

P26

Sputter-grown 2D-TI/3D-TI stacking films in the Bi-Te binary system

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Bilayer Bi is known as a 2D topological insulator [1], while Bi_2Te_3 is a representative 3D topological insulator [2]. Bi_2/Bi_2Te_3 (nominal composition of Bi_4Te_3) is a naturally formed superlattice that can be fabricated using sputtering, a technologically friendly technique. The obtained films showed strong orientation of the c-axis in the out-of-plane direction, indicating van der Waals gaps form parallel to the substrate surface and the in-plane grain size is about 30-40 nm [3]. High angle annular dark field-scanning transmission electron microscopy (HAADF-STEM) confirmed at atomic resolution the alternate Bi_2/Bi_2Te_3 stacking as shown in Fig.1(a). Since both Bi_2 and Bi_2Te_3 are layered crystal structures with the two constituent layers bonded via weak van der Waals interactions. Density functional theory calculations were carried out to ascertain the electronic band structure of Bi_4Te_3. The calculations showed that a Dirac cone occurs at the Gamma point only when spin-orbit coupling (soc) is included in the calculation (Fig.1(d)-(f)). These results suggest that Bi_4Te_3 is topologically non-trivial. The presence of a Dirac cone even in the bulk will make this material promising for future electronics and spintronics applications.

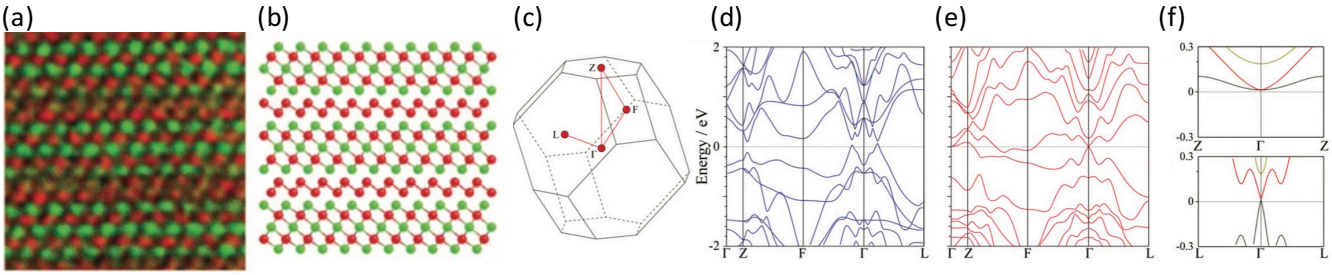

FIG. 1. (a) HAADF-STEM image. Bi and Te atoms are represented in red and green, respectively. (b) Crystal structure of Bi_4Te_3. (c) Schematic image of the Brillouin zone. Calculated band structure (d) without soc and (e) with soc. (f) Detailed band dispersions around the Gamma point.[3]

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P27

Topological transport in noncollinear antiperovskites

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Antiferromagnetic (AFM) spintronics has recently become a hot research topic. In comparison to ferromagnets, AFM materials are robust against perturbations due to magnetic fields and enable faster switching frequency in the THz range. Non-collinear magnetic compounds, as one important class of AFM materials, have also attracted intensive attention and more specifically, Mn_3X systems with X = Sn,Ge,Ga,Ir, and Rh have been proposed to host large intrinsic anomalous Hall conductivities [1],[2]. In this work, we performed first-principles calculations on the non-collinear antiperovskite Mn_3GaN to investigate the behavior of the anomalous Hall conductivity (AHC) with respect to the magnetization direction. Our results reveal that the AHC displays a significant dependence with respect to the in-plane magnetization direction between the Γ_{5g} and Γ_{4g} magnetic configurations where large anomalous Nernst effect can be induced by tailoring the magnetization direction. Moreover, we observed strong piezospintronic effect in Mn_3GaN, where large AHC can be induced by moderate epitaxial strain. Symmetry analysis reveals that for both cases, the nonzero anomalous Hall conductivity is originated from the spin-orbit coupling instead of the noncollinear magnetic configurations. Finally, we performed systematic high throughput screening for magnetic cubic antiperovskites, and studied the magnetic ground state and the piezospintronic effect for those compounds with noncollinear magnetic structure.

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P28

Impact of Ultrafast Transport on the High-Energy States of a Photoexcited Topological Insulator

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Ultrafast dynamics in three-dimensional topological insulators (TIs) opens new routes for increasing the speed of information transport up to frequencies thousand times faster than in modern electronics. However, up to date, disentangling the exact contributions from bulk and surface transport to the subpicosecond dynamics of these materials remains a difficult challenge. Here, using time and angle-resolved photoemission, we demonstrate that driving a TI from the bulk-conducting into the bulk-insulating transport regime allows to selectively switch on and off the emergent channels of ultrafast transport between the surface and the bulk. We thus establish that ultrafast transport is one of the main driving mechanisms responsible for the decay of excited electrons in prototypical TIs following laser excitation. We further show how ultrafast transport strongly a?ects the thermalization and scattering dynamics of the excited states up to high energies above the Fermi level. In particular, we observe how inhibiting the transport channels leads to a thermalization bottleneck that substantially slows down electron-hole recombination via electron-electron scatterings. Our results pave the way for exploiting ultrafast transport to control thermalization time scales in TI-based optoelectronic applications, and expand the capabilities of TIs as intrinsic solar cells.

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Multistage chemical bath deposition of thick film cadmium sulfide for CdS/CdTe X-ray detector

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Abstract

Many methods are used to measure X-ray flux generated by modern X-ray machines. The most common method utilized for monitoring X-ray dose is technically complex and expensive. In this work multilayer of cadmium sulfide (CdS) using chemical bath deposition (CBD) were carried out to deposit thick layer optimum thickness to produce CdS/CdTe junction x-ray detector. The effects of the deposition time, cadmium chloride heat treatment, the ammonia and thiourea concentration on CdS layers were controlled and investigated through scanning electron microscope (SEM), energy dispersive x-ray analysis (EDXA), X-ray diffraction (XRD), and ultraviolet (UV)-visible spectroscopy. The XRD analysis showed that the CdS films have highly oriented crystallites with the classical hexagonal structure (wurtzite type) and the main six diffraction peaks. The relatively stronger and narrow peak of CdS film obtained with 6 stages along (002) plane indicated that the film is highly oriented along the c-axis. The band gap Eg can be extrapolated to be 2.41 eV. It was observed that the maximum and the minimum amplitudes of the pulse formed due to exposed FTO/CdS/CdTe/Mo detector to Xray of 33 keV and 1mA intensity are 0.732 and -0.405 V and consequently the total output amplitude is 1.137 V. Keywords: CdTe; CdS; Thin film; X-ray; Detector

P30

Effect of Deformation on the Electronic Structure and Topological Properties of the $A^{II}Mg_2Bi_2$ (A^{II} = Mg, Ca, Sr, Ba) Compounds

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Recently, much attention has been paid to the study of the properties of topological insulators and Dirac semimetals, which are of interest primarily due to their electronic structure features near the Fermi level. The band structure of the surface of a topological insulator includes a Dirac cone formed by two spin-polarized bands with linear dispersion intersecting at the Dirac point at the Fermi level. In this case, the fundamental energy gap of the bulk material is inverted near certain high-symmetry points of the reciprocal space (so-called TRIM points). A Dirac semimetal is characterized by the presence of the Dirac cone formed by doubly degenerate bands in the band structure of the bulk crystal. Due to their exotic properties, these materials are promising in terms of their use in electronic devices of a new generation. Consequently, the search for compounds with such properties is an actual task for creation of the elemental base of new electronics.

We present the results of an initial theoretical study of the electronic structure and topological properties of the $A^{II}Mg_2Bi_2$ (A^{II} = Mg, Ca, Sr, Ba) compounds in the equilibrium state, under the hydrostatic pressure and uniaxial deformation.

It has been shown that the Mg_3Bi_2 compound in the equilibrium state is a semimetal, whereas the $CaMg_2Bi_2$, $SrMg_2Bi_2$ and $BaMg_2Bi_2$ compounds are semiconductors with a direct fundamental band gap. In the case of hydrostatic pressure in the three-component compounds, we have revealed a semiconductor–semimetal transition without change in the topological properties. Uniaxial tension of the $CaMg_2Bi_2$, $SrMg_2Bi_2$ and $BaMg_2Bi_2$ compounds results in the transition from the semiconductor to the Dirac semimetal phase. Uniaxial compression leads to a richer spectrum of the observed electron phases. In the $CaMg_2Bi_2$ compound, the semiconductor–topological insulator–topological semimetal sequence is realized, in the $SrMg_2Bi_2$ compound the semiconductor–Dirac semimetal–topological insulator–topological semimetal, and the $BaMg_2Bi_2$ semiconductor–topological insulator. Therefore, it becomes possible to control topological properties of the $CaMg_2Bi_2$, $SrMg_2Bi_2$ and $BaMg_2Bi_2$ compounds by uniaxial tension or compression. In the case of the Mg_3Bi_2 compound, none of the deformations considered leads to qualitative changes in the band structure and topological properties. Owing to the rich spectrum of topologically nontrivial phases, the compounds $CaMg_2Bi_2$, $SrMg_2Bi_2$ and $BaMg_2Bi_2$ may be of interest for further theoretical and experimental studies [1].

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P31

Bound states of Dirac electrons on the Bi_2Se_3 surface

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On the surface of the topological insulator Bi_2Se_3 in the vicinity of steps and other extended defects band bending occurs, leading to the formation of potential wells for the surface electrons. We present results of ultra-high vacuum scanning-tunneling spectroscopy investigation of local density of states in such wells. We demonstrate here, that bound states of massless Dirac electrons are formed in the potential wells near the surface steps and other linear defects of the surface.

As shown earlier [1], on the Bi_2Se_3 surface in the vicinity of steps and other extended defects on a ~ 10 nm scale a $100-200$ meV band bending occurs, which means that potential wells for the surface electrons are formed. In the present work results of ultra high vacuum scanning tunneling spectriscopy (UHV STS) investigation of local density of states (LDOS) in such wells are presented. We find, that bound states of massless Dirac electrons are formed in the observed potential wells. Comparison of the experimental data with the numerical simulation results supports this conclusion.

In Fig. 1(a) results of spatially resolved scanning tunneling spectroscopy in the vicinity of a linear defect (a protrusion of height 0.12 nm and width ~ 10 nm) are presented. Such defects presumably correspond to buried grain boundaries (see, for example, [2]). White dashed lines represent the Dirac point position and the approximate positions of the bulk band edges. The potential landscape in the area of the defect comprises a potential well of depth $U \approx 0.7$ eV and width $l \approx 10$ nm. At $V \approx -0.18$ V a horizontal maximum appears, localized in the potential well, which hints at the existence of a bound state.

Similar features are obsrved near steps on the Bi_2Se_3 surface. Potential wells for the surface electrons are formed due to the band bending on a ~ 10 nm scale a $100-200$ meV in the vicinity of surface steps [1]. In Fig. 1(b) a tunneling spectrum taken in such a quantum well in the vicinity of a step is shown. We see that the differential tunneling conductance curve changes substantially inside the well. Namely, the V-shaped minimum, representing the Dirac cone apex, flattens out, becoming a plateau, on the side of which the differential tunneling conductance grows rapidly and a peak is formed.

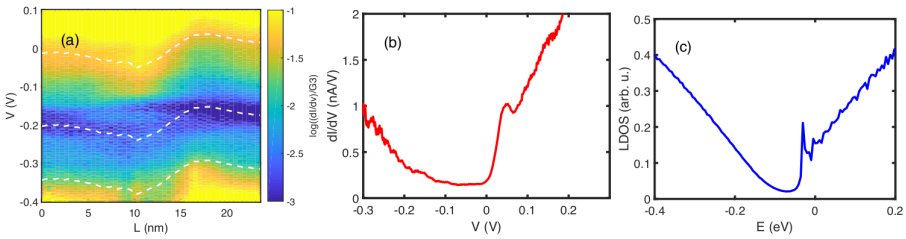

FIG. 1. (a) LDOS distribution obtained from STS on line across a linear defect on the Bi_2Se_3 surface. White dashed lines represent the Dirac point position and the approximate positions of the bulk band edges. (b) LDOS in a potential well on the Bi_2Se_3 surface obtained from STS and (c) numerical simulation results for a Gaussian potential well $U(x) = U_0 \exp(-x^2/2x_0^2)$, $U_0 = 0.1$ eV, $x_0 = 7$ nm.

To investigate the effect of the potential well on the topologically protected surface states and in particular the possibility of bound states formation, we perform numerical calculations of the local density of states in the vicinity of the extended defects on the Bi_2Se_3 surface by using a model Dirac Hamiltonian $H = A\boldsymbol{\sigma}\boldsymbol{k} + U(x)$ with a 1D potential well $U(x)$. Here $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ is the Pauli matrices vector, $\boldsymbol{k}$ is the wave vector of the surface electrons, $A \approx 0.3$ eVnm is the Fermi velocity. We employ a finite difference method to solve the corresponding equation.

In Fig. 1(c) a calculated local density of states curve in a Gaussian quantum well is shown. We see that the main features of the tunneling spectrum in Fig. 1(b), namely the disappearance of the V-shaped minimum at the Dirac point and the emergence of a plateau and a peak, are reproduced. Further analysis shows, that, in the framework of the model considered, states, localized in the x-direction (perpendicular to the potential well), arise and make a substantial contribution to the peak in the local density of states.

We also simulate the spatial distribution of surface states LDOS and compare it to the experimental STS results. We use known for Bi_2Se_3 parameters of the surface states and an approximation of the potential landscape from experimental results obtained on a step as well as on a linear protrusion on the surface of Bi_2Se_3. In both cases both energy and spatial distribution of the calculated LDOS are in reasonable agreement with the experiment.

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P32

Optical and elastic properties of the topological insulator $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$: Role of bulk defects

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Recently, the quaternary $Bi_{2-x}Sb_xTe_{3-y}Se_y$ compound has exhibited pronounced topological surface states with an insulating bulk [1–4]. It was found that, at (x,y)=(0.5,1.3) ($Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$), the electron and hole carriers compensation is maximally realized. The bulk-insulating behavior in the $Bi_{2-x}Sb_xTe_{3-y}Se_y$ solid solution is achieved by introducing two prevailing types of charged defects, such as (Bi,Sb)/Te antisite defects and the Se vacancy defects [1]. However, other defects can also be formed. To characterize the bulk defects in the topological insulators non-destructive local probes, which should be performed on the same sample, are needed, because the presence of point defects in the sample depends on the growth conditions and their random distribution across the crystal is difficult to control. In this report, we present the experimental studies of the optical, elastic and structural properties of the $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ single crystal and compare them to those to binary tetradymite Bi_2Te_3.

High-quality $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ and Bi_2Te_3 single crystals were grown by the modified Bridgman technique with a temperature gradient of about 10 K·cm^{-1} at the front of crystallization [5]. The crystal structure of $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ and Bi_2Te_3 samples was determined using the X-ray powder diffraction with diffractometer Shimadzu XRD 7000 Maxima (Cu Kα-radiation, graphite monochromator, scattering angle range $2\vartheta = 15^\circ - 71.5^\circ$ at room temperature, and $20^\circ - 70^\circ$ at lower and higher temperatures). The samples patterns are essentially the same and can be well indexed with the rhombohedral structure, confirming that the $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ maintains the same crystal structure as Bi_2Te_3.

We found the anomalous behavior of the elastic and optical properties in $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ that is absent in Bi_2Te_3. The extra vibrational excitation was observed in the Raman spectrum near 125 cm^{-1}. Its line width has increased substantially with the increasing temperature, and its frequency showed a sharp softening in the temperature range of 200-250 K. In the same temperature range, a large peak in attenuation of longitudinal ultrasound wave propagating along the trigonal axis and the step-like anomaly on the temperature-dependence of elastic modulus C_{33} were found. We revealed a correlation between the anomalous behavior of the elastic and optical properties and suggested that they are of a common nature and caused by bulk defects with a low symmetry. These defects are most likely located in the upper Te/Se and Bi/Sb quintuple layers, the most suitable ones are pairs: Se interstitial+(Bi,Sb)/Te antisite defects. The activation energy of the defect of 78 meV determined from the temperature dependence of the relaxation time is likely to represent the thermal barrier for hopping processes. The importance of our results is in the identification of a new type of defects in $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$, which can affect the transport, thermoelectric and other properties not only in the bulk, but also on the surface of three-dimensional topological insulators.

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P33

Topological quantum phase transition from mirror to time reversal symmetry protected topological insulator

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Topological insulators constitute a new phase of matter protected by symmetries. Time-reversal symmetry protects strong topological insulators of the Z_2 class, which possess an odd number of metallic surface states with dispersion of a Dirac cone. Topological crystalline insulators are less robust and merely protected by individual crystal symmetries. They show an even number of Dirac cones. In this work, it is demonstrated that Bi doping of $Pb_{1-x}Sn_xSe$ (111) epilayers induces a quantum phase transition from a topological crystalline insulator to a Z_2 topological insulator. This occurs because Bi-doping lifts the fourfold valley degeneracy and induces a gap at Γ, while the three Dirac cones at the M points of the surface Brillouin zone remain intact. We interpret this new phase transition as caused by a lattice distortion. It implies that the system becomes ferroelectric. Our results demonstrate that strong topological insulators can be switchable by distortions or electric fields.

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