P-2019b. Investigation of electronic structure of the magnetic-doped topological insulator TlBi0.9Gd0.1Se2

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Introduction

Investigation and modification novel solid state systems are of interest in both of fundamental and applied research. Time-reversal symmetry (TRS) protected topological insulators (TIs) are one of the such systems that possess unique spin-locked topologically protected surface states (TSS) located in the bulk band gap. These surface states are described by linear dispersion forming the spin polarized Dirac cone. In heart of extraordinary properties lies band inversion at the Γ – point originated from strong spin-orbit coupling (SOC)[1-4].

One of the trends in study of such systems is investigation interaction of TSS and magnetic field. Magnetic order breaks TRS lifting of Kramers degeneracy between opposite spin-oriented states which leads to opening a band gap at the Dirac point. Theoretically, it is justified that such behavior of the electronic structure can produce a lot of fundamentally and applied significant effects. Such phenomena like topological magnetoelectric effect, quantum anomalous Hall effect (QAHE) and the possibility of magnetic monopoles observation are expected to be observed in magnetic TIs. Furthermore, based on TRS-broken TIs, there are many concepts of spintronics devices construction, e.g. a spin transistors. Possible ways to create a magnetic order in TIs are doping by transition or rare earth metals, proximity effect with magnetic layer or growing a stoichiometric magnetic system. Thus, study of chromium [5] and vanadium [6] doped TIs made it possible to achieve QAHE regime transition at extremely low temperatures - 30 mK and 130 mK, respectively. Investigation of manganese based stoichiometric TI MnBi2Te4 revealed antiferromagnetic order bellow 25K and magnetic gap at the Dirac point [7]. Although, exist a lot of outstanding problems worthy of further study. Firstly, it is very low temperatures of QAHE regime transition for Cr- and V- doped systems, which make it difficult to implement to applied engineering. On the other hand, gap at the Dirac point does not always have a magnetic nature. In addition to magnetism, a number of other factors, e.g. impurity scattering coupled with dephasing on non-magnetic atoms, scattering on potential of magnetic atoms or even Higgs-like mechanism can open a gap at the Dirac point but do not contribute to observing the above effects. Hereby, discussions about existence of a gap at the Dirac point and its origin are one of the most investigating topics in the TIs research area over the past years. Our study is focused on electronic and magnetic structures investigation of gadolinium (Gd) - doped TI TlBi0.9Gd0.1Se2. Previously, Gd-doped Bi(Sb)2Se(Te)3 TIs were studied demonstrating antiferromagnetic or paramagnetic order.

Further, in the paper [9] we have shown that Gd-doped TI Bi1.09Gd0.06Sb0.85Te3 have unique electronic and magnetic structure with ferromagnetic hysteresis at 100K which disappears with temperature decreasing. That effect can be related with two dimensional surface magnetism via TSS - RKKY like mechanism. However we did not observe significant gap at the Dirac point by means of angle resolved photoemission spectroscopy (ARPES), which possibly related with small percentage of doping and small Zeeman splitting. Thus, studying the effect of Gd on the magnetic and electronic structures of TI seems to be a promising task. At the present, we aimed on study Gd atoms impact on electronic structure of thallium based TI TlBiSe2. Thallium based

topological insulator TlBiSe2 was theoretically and experimentally investigated demonstrating promising electronic structure with the largest value of bulk band gap among to three dimensional TIs as well as existence of linear dispersion surface states within the band gap. Distinctive feature of such kind of TIs is absence of van der Waals gap between atomic layers in perpendicular to the surface direction (0001) which may influence on magnetic properties in case of doping with magnetic atoms. Here we present the first investigation of electronic and magnetic structure of gadolinium doped thallium based topological insulator with stoichiometry TlBi0.9Gd0.1Se2 by angle-/spin- resolved photoemission spectroscopy and superconducting interference magnetometry.

Results and discussion

Magnetic characterization

Before start to study electronic structure we carried out magnetic characterization using SQUID magnetometry. In Fig. 1 (b) the dependencies of magnetization per mole as a function of applied out-of-plane magnetic field (B||C) measured for TlBi0.9Gd0.1Se2 with SQUID magnetometer at different temperatures is shown. The dependence measured at temperature of 2K demonstrates the well known S-like characteristic for paramagnetic or antiferromagnetic behavior. The temperature dependence of magnetic susceptibility in an applied out-of-plane field of 0.1 T is presented in Fig.1(c). Here, one can see the approximation of the dependence by the Curie-Weis law ($x = \frac{C}{(T-\theta)}$), where C is the material specific constant and θ is the Weiss temperature). The fitting by linear function gives a Weiss temperature equal to zero, that points forward for paramagnetic order in such material.

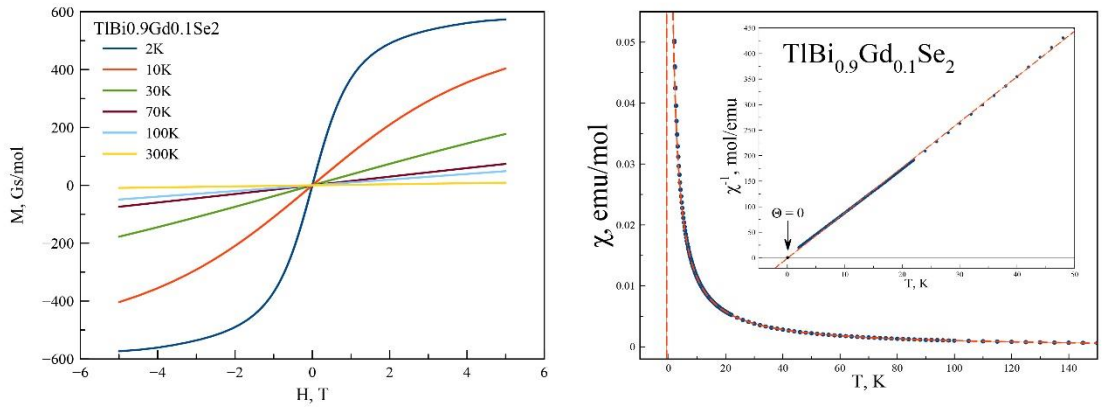

Fig. 1, (a) Magnetic field dependences of the effective magnetization at different temperatures. (b)Temperature dependence of the magnetic susceptibility and inverse temperature dependence of the magnetic susceptibility of the sample. Measurement were carried out in in the resource center "Center for Diagnostics of Materials for Medicine, Pharmacology and Nanoelectronics" of the SPbU Science Park using a SQUID (Superconducting Quantum Interference Device) magnetometer with a helium cryostat manufactured by Quantum Design.

In the meanwhile, one can see that dependencies of magnetization per mole as a function of applied out-of-plane magnetic field at 2K does not reach saturation, that can be result of weak antiferromagnetic interaction between magnetic atoms. In additional, two important fitting parameters of C, which are related with the effective magnetic moment and θ - Weiss temperature can be calculated from the linear plots of $\frac{1}{x}$ in the high temperature range. From this analysis, the reasonable effective magnetic moment of μ_{eff} = 8.0 μB per Gd atom was found. Such μ_{eff} value

is equal to the theoretical value of 8.0 μB expected for free Gd^{3+} ions. These results indicate that the gadolinium atoms are effectively well substituting bismuth. It should be noted that in our previous work we observed antiferromagnetic order in Bi1.09Gd0.06Sb0.85Te3 at much higher temperature – near 8.3 K despite on lower Gd-concentration. We relate such behavior with different crystal and electronic structure of the samples. In case of RKKY interaction - which is more likely for Gd as dopants in 3D TI, value of interaction decrease with increase of wave vector on Fermi level (k_f). Here we have relative large and, consequently, - low temperature of antiferromagnetic transition. Furthermore, we do not see a hysteresis at elevated temperatures, which is also could be related with absence of van der Waals gap and as a consequence such material can not be considered as a system consisting of quasi-two- dimensional layers in which its own magnetic order can form.

Electronic structure

To investigate electronic structure of TSS in TlBi0.9Gd0.1Se2 we carried out laser based ARPES measurement. In Fig.2 (a, b) ARPES images measured at the Γ point region with using different linear polarization of laser radiation are presented. One can see that electronic structure near the Fermi level characterized by the clearly seen Dirac cone with absence of valence and conducting band states near the Dirac point region. In Fig. 2 (c) and in Fig. 3 CDARPES image measured at the Γ point is shown. One can see that different branches have opposite sign of CDARPES asymmetry which partly prove helical spin structure of the sample. Hereby, electronic structure near the Fermi level of TlBi0.9Gd0.1Se2 is characterized by Dirac cone with helical spin structure near the Γ - point.

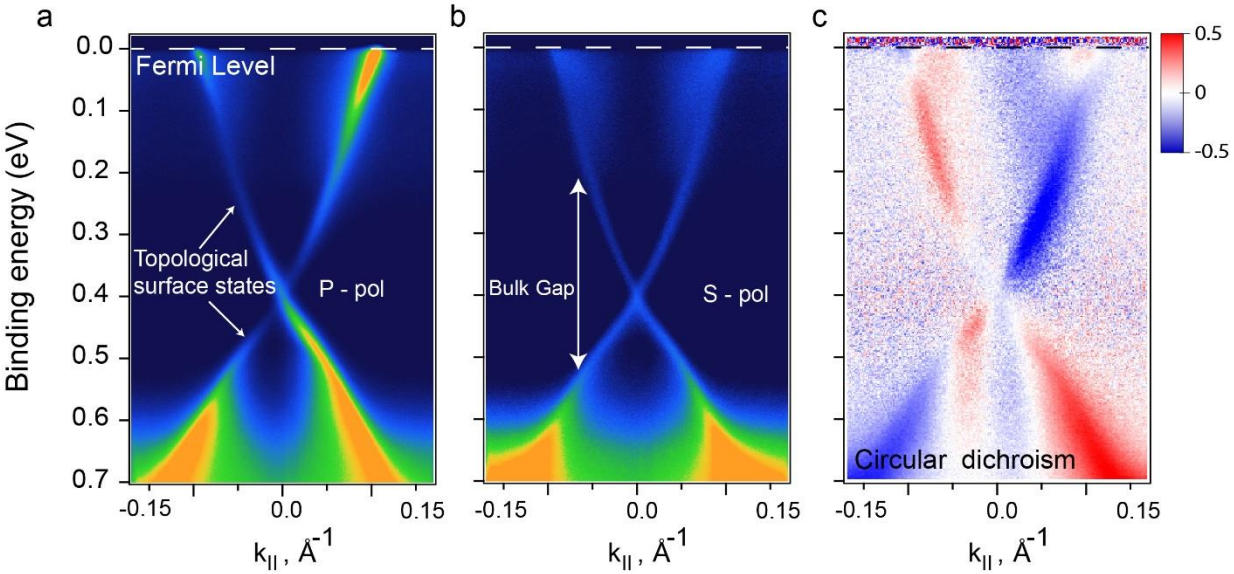

Fig. 2, (a) FIG. 2. ARPES images for TlBi0.9Gd0.1Se2 measured near the point using laser radiation with di erent polarization. Photon energy = 6.3 eV, temperature = 15 K.

Even though a paramagnetic phase is not characterized by its own total magnetic moment other than zero, opening of a magnetic gap at the Dirac point can still be expected. Previously, the gap about 25 meV in TSS for gadolinium and vanadium doped TI above the Neel temperature was reported [8]. In manganese based stoichiometric TI MnBi2Te4, gap at the Dirac point was also found even above the Neel temperature [7]. At the moment several mechanisms for the formation of a gap at the Dirac point above temperature of magnetic ordering were proposed, for example, asymmetric spin generation in the process of photoemission [8] or spin fluctuations [7]. In Fig.3 (a) laser based ARPES image measured with using s-polarized light with more detailed analyze of the Dirac cone behavior near the point is presented. At the right panel, zoomed second derivative with respect to the energy of the band dispersion is shown. One can see existence of a small gap at this image. We estimated gap size of 20 meV (estimations shown by white dotted line). Also,

electronic structure near the Fermi level was measured by synchrotron radiation with different photon energy. In Fig.3 (b) one can see ARPES images of TSS measured by s-polarized synchrotron radiation and excitation energy of 18 eV. One can see that size of gap at the Dirac point directly depends on photon energy - 50 meV according to our estimates for synchrotron radiation. Additionally, synchrotron photon energies allow us to estimate the bulk band gap as 0.3 eV, in agreement with the previous studies of thallium based TIs [35]. It should be noted that all measurements were made with precise calibration at the Γ point. Before every measurement we did k_x, k_y mapping to exclude any misalignment. Actually, we can not clear explain this feature and it will be a goal of the future tasks.

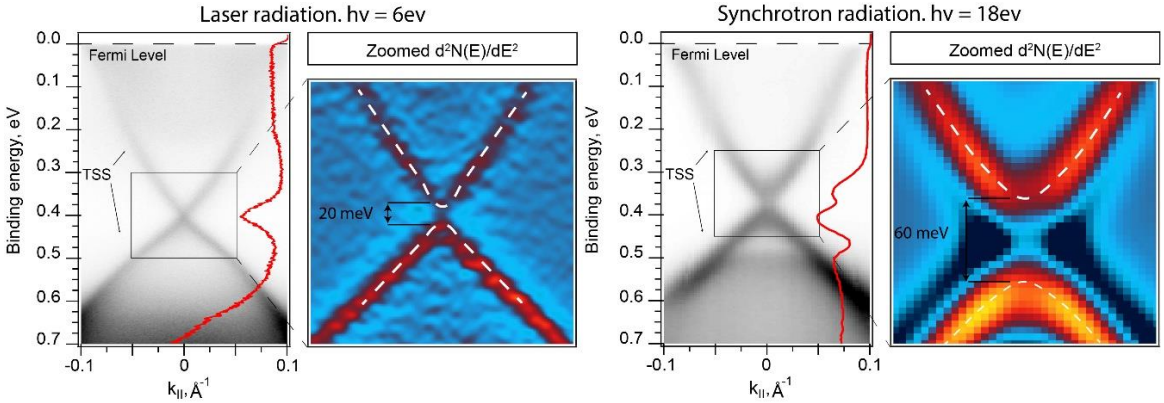

FIG. 4. (a) ARPES images for TlBi0:9Gd0:1Se2 measured near the □ point using laser radiation. Photon energy = 6.3 eV, temperature = 15 K. (b) The same type of image but measured by using the synchrotron radiation. Photon energy = 18 eV, temperature = 15 K. Near with both of ARPES images second derivative from intensity to energy zoomed at the Dirac point region is shown. Energy distribution curves at the Dirac point presented by red line.

Conclusion

In conclusion, we have experimentally investigated magnetic and electronic structure of Gd-doped topological insulator TlBi0.9Gd0.1Se2. SQUID measurement revealed paramagnetic order up to 2 K. Electronic structure measured by angle resolved photoemission spectroscopy with different polarization of light revealed existence of high quality topological surface state with helical spin structure located in the bulk band gap. Analysis of the Dirac cone near the Γ point shown possible existence of a gap at the Dirac point even at paramagnetic phase. Furthermore, we observed that size of a gap at the Dirac point strongly depends from photon energy.

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Personal experience

Even though I was able to stay in Berlin for only 2 weeks, it was a very busy period. In the first week, Alexander Fedorov and Vova Voroshnin and I were engaged in the synthesis of graphene and assembled a chamber for MBE. The second week we were engaged in measuring the electronic structure of the above sample. It was the end of September and there was a frost in Berlin, perhaps thanks to this we were able to get such a good data

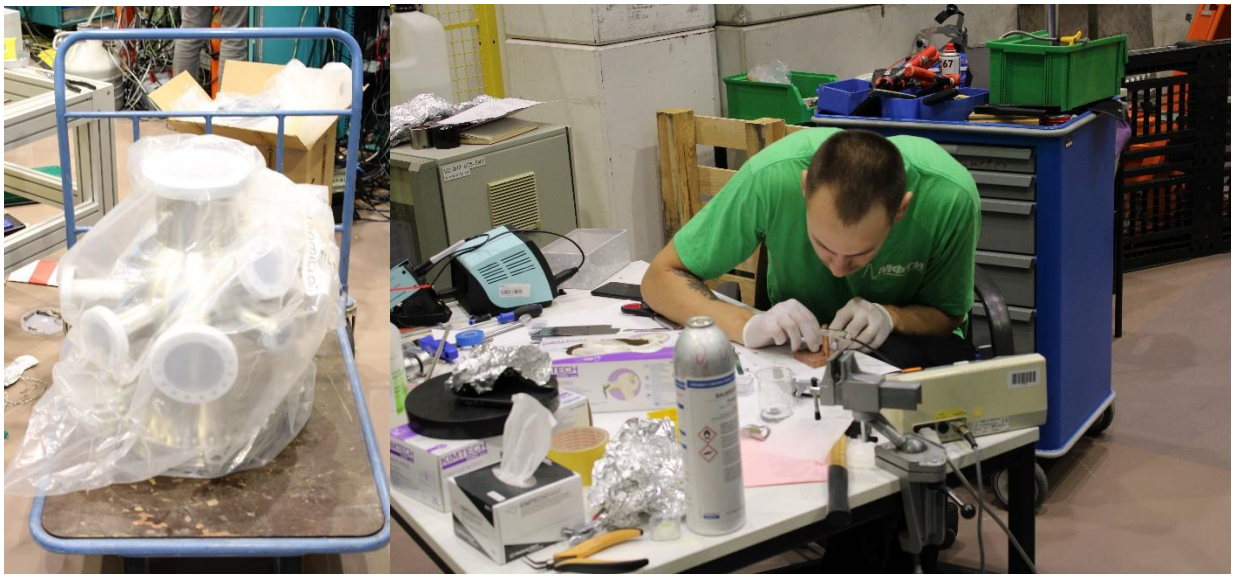

Fig.4 a - *some kind of important thing with holes for MBE chamber. b- me trying to cope with a welding machine*