

Contents

Certificate	iii
Declaration by the Candidate	v
Copyright Transfer Certificate	vii
Acknowledgements	ix
Contents	xv
List of Figures	xviii
List of Tables	xxv
Preface	xxvii
Chapter 1: Introduction: A bibliographic review	33-56
1.1 Introduction	35
1.2 Topology in geometry	38
1.3 The concept of Topology in integer quantum Hall effect	39
1.4 The tour from quantum hall to quantum spin hall effect	40
1.5 Topological Insulator to Topological Semimetals	43
1.4.1 Weyl Semimetals	46
1.6 Magnetic Topological materials	49
1.6.1 Quantum oscillation	53
1.7 Topological Insulator under Pressure	54
1.7.1 Crystal structure and Symmetry Properties under pressure	56
Chapter 2: Methodology and Characterization tools	57-76
2.1 Introduction	59
2.1.1 Modified Bridgeman technique	59
2.1.2 Chemical vapour transport technique	60
2.2 Experimental characterization tools	61
2.2.1 X-Ray diffraction (XRD)	61
2.3 Transport property measurements	63
2.3.3.1 Electric resistivity (ρ_{xx})	63
2.4 Magnetic property measurement System (MPMS)	67
2.4.1 DC magnetization and AC susceptibility	67
2.5 Raman Spectroscopy	69
2.6 High Pressure Techniques	71
2.7 Fundamentals of ARPES	73
2.8 Theoretical DFT	76
Chapter 3: Defect induced Ferromagnetic Ordering and Room Temperature Negative Magnetoresistance in MoTeP	77-96
3.1 Introduction	79
3.2 Methods	80
3.2.1 Structural Characterization	80
3.2.2 Material Characterization	80
3.2.3 DFT	81
3.3 Results and discussions	81

Contents

3.3.1 Zero field resistivity behaviour	81
3.3.2 Hall effect study	83
3.3.3 Magnetic behaviour	86
3.3.4 Effect of magnetic field on longitudinal resistivity	87
3.3.5 DFT calculation	92
3.3.6 Temperature dependent Raman measurements	95
3.4 Conclusion	95
Chapter 4.A: Experimental and Theoretical Revelation of a Unique Band Topology in Sb_2Te_3 Topological Insulator by substitution of Cu- A High Pressure Study	97-115
4.A.1 Introduction	99
4.A.2 Methods	101
4.A.2.1 Computational details	101
4.A.3 Results and Discussion	101
4.A.3.1 XRD	101
4.A.3.2 Raman measurements	109
4.A.3.3 Theoretical discussions	112
4.A.4 Conclusions	114
Chapter 4.B: Pressure induced topological and structural transitions in iron and sulphur doped Sb_2Te_3	117-124
4.B.1 Introduction	119
4.B.2 Results and Discussions	119
4.B.3 Conclusion	124
Chapter 5: Above-Ordering-Temperature Anomalous Hall Effect in A Rare Earth Doped Topological Insulator BiSbTe_3	125-146
5.1 Introduction	127
5.2 Methods	129
5.3 Results and Discussion	129
5.3.1 XRD	130
5.3.2 Resistivity behaviour	130
5.3.3 Field effect on longitudinal resistivity	131
5.3.4 Hall study	132
5.3.5 Magnetic behaviour	137
5.3.6 sdH oscillation	144
5.4 Conclusions	145
Chapter 6.A: Unusual Double Glassy phase and Anomalous Hall effect in S-doped (SbFe)$_2\text{Te}_3$ Topological Insulator	147-166
6.A.1 Introduction	149
6.A.2 Results and Discussions	150
6.A.2.1 XRD	150
6.A.2.2 Resistivity behaviour	151

Contents

6.A.2.3 Magnetic behaviour	153
6.A.2.4 ac susceptibility	157
6.A.2.5 Temperature dependent Raman	163
6.A.2.7 dHvA oscillation	164
6.A.2.7 ARPES	166
Chapter 6.B: Unusual Double Glassy phase and Anomalous Hall effect in S-doped (BiFe)₂Te₃ Topological Insulator	167-180
6.B.1 Results and Discussions	169
6.B.1.1 XRD	169
6.B.1.2 Resistivity behaviour	169
6.B.1.3 Magnetic behaviour	170
6.B.1.4 ac susceptibility	173
6.B.1.5 Temperature dependent Raman	177
6.B.1.6 ARPES	179
6.B.2 Conclusion	179
Chapter 7.A: Unusual Double Glassy phase and Anomalous Hall effect in S-doped (SbFe)₂Te₃ Topological Insulator	181-190
7.A.1 Introduction	183
7.A.2 Methods	184
7.A.3 Results and Discussions	184
7.A.4 Conclusion	190
Chapter 7.B: Unusual Double Glassy phase and Anomalous Hall effect in S-doped (BiFe)₂Te₃ Topological Insulator	191-200
7.B.1 Introduction	191
7.B.2 Methods	194
7.B.3 Results and Discussions	194
7.B.4 Conclusion	200
Chapter 8: Summary and future perspectives	201-208
8.1 Summary	203
8.2 Future perspectives	205
8.3 Applications	206
References	209-238
List of Publications	239
Schools / Meetings / Workshops / Conference Attended	240

List of Figures

Figure 1.1: Schematics of electronic bands in various solid-state materials. In semiconductors/insulators, the valence and conduction bands are separated by an energy gap. In metals, the valence and conduction bands overlap each other. In topological insulators, after band inversion, the valence and conduction bands are separated by the band gap, leaving behind conducting topological surface states in the form of linearly crossing Dirac cone. 35

Figure 1.2: Semiclassical description of integer quantum Hall state. 37

Figure 1.3: Geometrical objects with different topological classes represented by the genus numbers. 38

Figure 1.4: The interface between a quantum Hall state and an insulator has chiral edge mode. (a) The skipping cyclotron orbits. (b) The electronic structure of a semi-infinite strip described by the Haldane model. A single edge state connects the valence band to the conduction band. 40

Figure 1.5 Spatial separation is at the heart of both the quantum Hall (QH) and the quantum spin Hall (QSH) effects. (a) A spinless one-dimensional system has both a forward and a backward mover. Those two basic degrees of freedom are spatially separated in a QH bar, as illustrated by the symbolic equation “ $2 = 1 + 1$.” The upper edge contains only a forward mover and the lower edge has only a backward mover. The states are robust: They will go around an impurity without scattering. (b) A spinful 1D system has four basic channels, which are spatially separated in a QSH bar: The upper edge contains a forward mover with up spin and a backward mover with down spin, and conversely for the lower edge. That separation is illustrated by the symbolic equation “ $4 = 2 + 2$.” 41

Figure 1.6 (Color online) Edge and surface states of topological insulators with Dirac dispersions. (a) Schematic real-space picture of the 1D helical edge state of a 2D TI. (b) Energy dispersion of the spin non-degenerate edge state of a 2D TI forming a 1D Dirac cone. (c) Schematic real-space picture of the 2D helical surface state of a 3D TI. (d) Energy dispersion of the spin non-degenerate surface state of a 3D TI forming a 2D Dirac cone; due to the helical spin polarization, back scattering from k to $-k$ is prohibited. 43

Figure 1.7 Schematic illustration of Dirac node, Weyl node and Nodal line/ ring in momentum space. (a) Schematic of a Dirac semimetal where the bands are linearly dispersed around the Dirac point. The Dirac point is shown by the green dot. (b) Weyl semimetal, in which the Weyl points with opposite chirality are connected by the characteristic Fermi arc. The Weyl points are shown by the green dot and Fermi arc is shown by the black dotted line. (c) Nodal line semimetals where valence and conduction bands cross along special lines in momentum space forming either a ring-shaped line or 1D line, shown by the green circle/line. 45

Figure 1.8 (a) Dispersions for type-I Weyl fermion near E_F . The Weyl points (WP) are labelled by yellow and green dots, (b) Type-II Weyl semimetal with electron and hole pockets touching at two different energies, Crystal structures of MoTe_2 (c) in the $1T'$ and in (d) T_d phases. 47

List of Figures

Figure 1.9 (a) 3D bulk BZ and the projected (001) surface BZ of MoTe₂. Weyl points with positive and negative monopole charges are displayed as green and gray dots. (b) Calculated fine band structure of MoTe₂ along the K-K' direction crossing two types of Weyl points. (c) Calculated spectral intensity maps of MoTe₂ at E_F +5 meV. (d) Calculated spectral intensity maps of MoTe₂ at E_F (shifted by -0.02 eV to account for the slight hole doping). The white dashed boxes indicate the regions of interest shown in (c). (e) ARPES intensity maps of MoTe₂ measured at E_F with a 6.3 eV laser. (f), (g) ARPES intensity plot and the calculated electronic structure of Mo_{0.25}W_{0.75}Te₂ at k_x ~ k_w along the k_y direction. The red lines indicate the energy positions of the surface band bottom, the W1 point, and the W2 point, respectively. 49

Figure 1.10: Five mono atomic planes of a quintuple layer of Bi₂Te₃/Sb₂Te₃. 55

Figure 1.11 Schematic crystal structures of Sb₂Te₃ polymorphs: (a) α-Sb₂Te₃; (b) β-Sb₂Te₃; (c) γ-Sb₂Te₃ and (d) δ-Sb₂Te₃. 56

Figure 2.1: (a) Photograph of cleaved crystal sample, (b) schematic of CVT technique. 60

Figure 2.2: (a) Schematic of x-ray diffraction by crystallographic planes (b) Image of Rigaku Mini Flex II DESKTOP lab based XRD set up. 62

Figure 2.3: Schematic for (a) longitudinal resistivity measurements using four-probe geometry and (b) Hall resistivity measurements using four-probe geometry. The magnetic field is applied orthogonally to the applied electric current (I). 65

Figure 2.4: The Physical property measurement system (PPMS) set up at UGC-DAE, Kalapakkam node. 66

Figure 2.5: Van der Pauw contact configuration for measuring the resistivity: **upper panel**-longitudinal resistivity (MR), **lower panel**- transverse resistivity (Hall). 67

Figure 2.6: (a) Image of Quantum Design MPMS3 of CIFIC, IIT (BHU), (b) Schematic diagram of SQUID-VSM detection system. 68

Figure 2.7: (a) Energy-level diagram presenting the states involved in Raman scattering process, (b) Schematic diagram of Raman active vibrational modes. 70

Figure 2.8: Schematic of a diamond-anvil-cell (DAC) used for generating high pressure. 72

Figure 2.9: Schematic of ARPES measurements, **(b)** Energy and momentum dependence of the local density of states for (a)Sb₂Se₃, Sb₂Te₃, Bi₂Se₃, and Bi₂Te₃ on the [111] surface. The red and blue regions indicate bulk energy bands and bulk band gaps, respectively. The red lines, dispersing in the bulk gap around the Γ point, are the surface states. 75

Figure 3.1: **(a)** Thermal hysteresis of temperature dependent resistivity of 1T' MoTeP, **inset:** low temperature resistivity data, orange solid line is a fit of electron-electron and electron-phonon scattering terms $\rho(T) = \rho_0 + aT^2 + bT^5$, **(b)** temperature evolution of ρ_{xx} and $d\rho_{xx}/dT$ at zero magnetic field, **(c)** Field dependence of Hall data ρ_{xy} at various temperatures, **inset:** measurement geometry, **(d)** low- field low-temperature

List of Figures

conductivity data, solid orange line shows HLN fitting to $\Delta\sigma(e^2/h)$ at various temperatures. 82

Figure 3.2: (a), (b) Field dependence of Hall conductivity σ_{xy} and longitudinal conductivity σ_{xx} at 2,50,100 and 200K, orange solid lines are their respective two-carrier model fit with equations 1 and 3, (c) density of electrons n_e (black circle) and density of hole n_h (red circles) as a function of temperature extracted from σ_{xy} , **inset:** ratio of n_h and n_e as a function of temperature, (d) electron mobility μ_e (black circle) and hole mobility μ_h (red circles) and their ratio μ_h/μ_e , **inset:** as a function of temperature. 85

Figure 3.3: (a) Magnetic field dependent MR% at various temperatures ranging from 2K-300K, inset shows 2K MR% with a power law fit (orange solid line), (b) clear pictorial view of positive MR at low field and negative MR at high field for 300K data, **inset:** measurement geometry, (c) Kohler's scaling of MR% as a function of B/ρ_0 up to 300K, **inset:** Kohler plot on logarithmic scale up to 200K, (d) M-B magnetic hysteresis curve taken at 5K and 300K. 88

Figure 3.4: (a) Bulk band structure of T_d -MoTeP with inclusion of SOC, (b) Spin-resolved Total DOS for defect induced MoTeP. 92

Figure 3.5: (a) Mo-d band contribution in bandstructure. 93

Figure 3.6: (a)-(c) Te-p band contribution in bandstructure, (d)-(f) P-p band contribution in bandstructure. 94

Figure 3.7: **Figure 3.7** Temperature dependent Raman spectra during (a) cooling and (b) heating cycle. The newly obtained mode is noted by arrow at 117.63 cm^{-1} indicating the presence of T_d phase. 94

Figure 3.8 (a) Magnetic moment as a function of temperature in ZFC and FC cycle; (b) MFM image taken at room temperature with scan areas $5 \times 5 \text{ }\mu\text{m}^2$. 95

Figure 4.A.1: (a) ADXRD patterns collected at various pressures for $\text{Sb}_{1.9}\text{Cu}_{0.1}\text{Te}_3$. The new peaks are marked with arrows, for phases II (C2/m), III(C2/c), and IV(Im-3m), respectively, Rietveld full-profile refinements of the diffraction patterns collected on compression at (b) 0.26 GPa (Rhombohedral R-3m phase), Le-Bail refinements of the diffraction patterns (c) 9.8 GPa (Monoclinic C2/m phase) and (d) 16.77 GPa (Monoclinic C2/c phase) and (e) 31.48 GPa (disordered cubic Im-3m phase) the difference plot is given below. The difference plot is shown in blue. Background is shown as green and the vertical marks give the individual phases of sample, Cu and W. 102

Figure 4.A.2: (a) c/a ratio as a function of pressure for ambient rhombohedral (R-3m) phase, 3 different colors indicate slope changes at those regions, (b) The volume as a function of pressure for initial rhombohedral phase with error bars. The dashed lines are the fitting results according to the third-order Birch-Murnaghan (red) and Murnaghan (blue) EoS, (c) Pressure dependence of the volume per atom (V/atom) for all the four phases. 103

List of Figures

Figure 4.A.3: Fit of compressibility with universal equation of state; blue solid line is (a) fit with Vinet EOS, (b) fit with Holzapfel EOS. 106

Figure 4.A.4: (a) Bond length of Te2-Sb, Te1-Sb and Te2-Te2 as a function of pressure, (b) angle of succession Te1-Sb-Te2 vs pressure, (c) vertical distance between intra-layer and interlayer. 107

Figure 4.A.5: (a) Schematic of $\text{Sb}_{1.9}\text{Cu}_{0.1}\text{Te}_3$ at various phases I(R-3m), II(C2/m), III(C2/c), IV(Im-3m) with pressure. 108

Figure 4.A.6: Experimental Raman spectra of $\text{Sb}_{1.9}\text{Cu}_{0.1}\text{Te}_3$ at pressures (a) 0.1 MPa - 10 GPa, (b) 11.3 - 30 GPa, (c) Pressure dependence of the Raman frequencies, the vertical dashed lines are an estimation of the pressure at which the electronic and structural phase transitions occur, blue hollow square and green crossed circles are for one run, red solid squares and magenta solid circles are for another run of Raman measurements. 110

Figure 4.A.7: (a) Bulk bandstructure of $\text{Sb}_{1.9}\text{Cu}_{0.1}\text{Te}_3$ at 0 GPa, (b) 0.26 GPa; inset: magnifying view at Γ -point shown, (c) 2.87 GPa. The Fermi level is set to zero. 112

Figure 4.A.8: Projected DOS and inset: Total DOS at (a) 0 GPa, (b) 0.26 GPa and (c) 2.87 GPa. The Fermi level is set to zero. 114

Figure 4.B.1: Schematics of $\text{Sb}_{1.9}\text{Fe}_{0.1}\text{S}_{0.15}\text{Te}_{2.85}$ structures at different pressures: (a) ambient R-3m, C2/m above 8.9 GPa, C2/c above 14.1 GPa, and $\text{Im}\bar{3}m$ above 15.1 GPa, (b) Single crystal XRD of $\text{Sb}_{1.9}\text{Fe}_{0.1}\text{S}_{0.15}\text{Te}_{2.85}$. 120

Figure 4.B.2: (a) ADXRD of $\text{Sb}_{1.9}\text{Fe}_{0.1}\text{S}_{0.15}\text{Te}_{2.85}$ up to 32 GPa, (b) c/a anomaly with pressure: solid red circles show c/a anomaly with pressure, hollow circles show comparison with pure Sb_2Te_3 . 121

Figure 4.B.3: (a) Volume as a function of pressure for all 4 phases, (b) Universal equation of state $\ln H$ as a function of $1-X$, (c) Fitting of 3rd order Birch-Murnaghan EOS on rhombohedral phase. 122

Figure 5.1: (a) Single crystal XRD and inset: powder XRD with Le-Bail refinement of $(\text{BiSbDy})_2\text{Te}_3$, (b) Fitting of electron-electron interaction term $A+BT^n$ on the low temperature part of the resistivity data ρ_{xx} . 130

Figure 5.2: (a) Resistivity evolution with temperature in the range 2-300K (pink), the derivative of ρ_{xx} data exhibits a jump at 44.2K (green), (b) Hall data as a function of field at various temperatures ranging from 2-100K, (c) the extracted carrier density (n_e) and mobility (μ_e) as a function of temperature, (d) The anomalous Hall part after extracting the linear part from the total Hall data. 132

Figure 5.3: (a) MR% data with field at various temperatures 2K, 5K, 10K, 25K, 50K, 100K, (b) The fitting of MR% data with the Kohler's scaling $B/\rho_{xx}(0)$ scaling, (c) The variation of magnetization with field at various temperatures

List of Figures

2K,10K,50K,100K,150K, **(d)** The magnetization evolution with temperatures in ZFC and FC cycle. 134

Figure 5.4 (a) The schematic of the different skew scattering mechanism in a clean FM, spin glass and cluster glass systems, **(b)** The anomalous Hall conductivity as a function of longitudinal conductivity, $\sigma_{xy} \propto \sigma_{xx}$ scaling showing skew scattering behaviour, **(c)** the anomalous Hall angle as a function of temperature. 138

Figure 5.5: (a) The AC susceptibility **(a)** real part and **(b)** imaginary part as a function of temperature at different frequencies, **(c)** The anomalous and Hall conductivity as a function of temperature, **(c)** frequency vs T_f plot, the best fit shows Dynamic fitting, **(d)** frequency vs T_f plot, the red line shows VF fitting. 140

Figure 5.6: (a)The frequency dependence of freezing temperature plotted as a $\ln(\tau)$ vs $\ln(t)$, where reduced temperature $t = (T_f - T_{SG})/T_{SG}$, the red line represents the linear fit to extract $z\nu$ and τ , **(b)** $\ln(\nu)$ vs $1/T_f$, the red line denotes the Arrhenius fitting to extract the thermal activation energy E_A and characteristic attempt frequency f_0 , **(c)** T_f vs $100/\ln(f_0/f)$, the solid line represents the linear fit to evaluate E_A and intercluster interaction strength T_0 , **(d)** $\ln(\nu)$ vs $1/(T_f - T_0)$, the red line denotes the linear fit to extract the thermal activation energy E_A and τ_0 . 143

Figure 5.7 (a) Contour plot of σ_{xy} in the B–T space with the magnetic phase diagram consisting of the antiferromagnetic (AFM) and paramagnetic (PM) phases, **(b)** the bandstructure of Dy doped BiSbTe₃ system. 144

Figure 5.8:(a) FFT of the original resistivity ρ_{xx} vs $1/B$ data to extract the particular frequency of the oscillation, this particular frequency(50T) is proportional to the area of the Fermi, and **(b)** inverse FFT to obtain 50T frequency signal in time scale, red solid line shows Landau Fan diagram to extract the phase and frequency of the signal. 145

Figure 6.A.1: (a) Single crystal XRD pattern of Sb_{1.9}Fe_{0.1}So_{0.15}Te_{2.85}, **(b)**resistivity evolution with temperature at zero magnetic field, **(c)**MR% at 2K for B||I and B⊥I configuration, **(d)** Hall resistivity at 2K, 10K, 25K, 50K and 100K, **(e)** AHE effect at 2K, 10K, 25K, 50K and 100K, **(f)** density and mobility evolution with temperature. 151

Figure 6.A.2: (a) dc magnetization vs temperature for Sb_{1.9}Fe_{0.1}So_{0.15}Te_{2.85} measured between 2 and 350 K at 100 Oe, 0.1T, and 0.4T, **(b)** ZFC and FC curves for 100 Oe, **(c)** dM/dT for 100 Oe ZFC curve to obtain the transition temperatures from inflection points, **(d)** Field dependence of magnetization measured at different temperatures, Temperature dependence of the **(e)** real (χ') and **(f)** imaginary (χ'') components of the ac susceptibility measured at frequencies varying from 5 to 500 Hz. 153

Figure 6.A.3: (a) The ZFC and FC susceptibilities vs T measured at H = 0.1 T, **(b)** the log-log plot of the M(T) curve along with the linear fits at low temperature, **inset:** evolution of magnetization as a function of field at 2K for Sb_{1.9}Fe_{0.1}Te₃. 154

Figure 6.A.4: Temperature dependent **(a)** Raman spectra, **(b)** 3D plot to see the clear variation between different modes, **(c)**Temperature evolution of the Raman shift of the E_g mode, and **(d)** M1 mode of Sb_{1.9}Fe_{0.1}So_{0.15}Te_{2.85}. 157

List of Figures

Figure 6.A.5: Dynamic scaling (a), (b) and Vogel-Fulcher (c), (d) fits of the “ T_f vs f ” curve respectively for T_{f1} and T_{f2} for $Sb_{1.9}Fe_{0.1}S_{0.15}Te_{2.85}$. 159

Figure 6.A.6: (a) Time dependence of thermoremanent magnetization at 25 K for 0.1T cooling field and wait time of 100s. The solid line is the best fit for KWW function to the data, (b) powder XRD pattern and its Rietveld refinement for the sample $Sb_{1.9}Fe_{0.1}S_{0.15}Te_{2.85}$. 161

Figure 6.A.7: (a) dHvA oscillation in the M-H data at low temperature and high magnetic field, (b) FFT amplitude data on frequency scale at 2K & 5K, 5 frequencies $F_\alpha \sim 40T$, $F_\gamma \sim 60T$, $2 F_\alpha \sim 80$, $2F_\beta \sim 100T$, $3F_\beta \sim 150T$ indicating Fermi surfaces of the sample, inverse-FFT with the (c) 60T and (d) $\sim 150T$ data by using band- pass filter, Landau Fan diagram to obtain the frequency and phase. 165

Figure 6.A.8: Temperature dependent angle resolved photoemission spectra taken at (a) 20K, (b) 150K, and (c) 260K with Synchrotron source of 95eV. 166

Figure 6.B.1: (a) Single crystal XRD pattern, (b) resistivity evolution with temperature at zero magnetic field, (c) MR% at 2K, 5K, 10K, 25K, 50K, 100K, 200K for B||I configuration, (d) Hall resistivity at 2K, 10K, 25K, 50K, 100K and 200K, (e) AHE effect at 2K, 10K, 25K, 50K, 100K and 200K, (f) density and mobility evolution with temperature for $Bi_{1.9}Fe_{0.1}S_{0.15}Te_{2.85}$. 169

Figure 6.B.2: (a) Temperature dependent dc magnetization $M(T)$ measured at different applied fields (100 Oe and 0.1T) for ZFC and FC protocols, (b) dM/dT as a function of temperature, (c) Magnetization as a function of external magnetic field at $T=5$ K, 100K and 300K (d) real (χ') and (e) imaginary (χ'') components of the ac susceptibility measured at frequencies varying from 100 to 700 Hz, (f) time dependence of thermoremanent magnetization at 25 K for 0.1T cooling field. The solid line is the best fit for KWW function to the data for $Bi_{1.9}Fe_{0.1}S_{0.15}Te_{2.85}$. 171

Figure 6.B.3: (a) DC Magnetization measured in ZFC and FC protocol taken at 100 Oe. Inset: $M(H)$ at 2K and 300K (b) The log-log plot of the χ_{dc}^{-1} vs temperature at 100Oe, Inset shows the suppression of GP at higher field (1000 Oe) for $Bi_{1.9}Fe_{0.1}Te_3$. 172

Figure 6.B.4: Dynamic scaling (a), (b) and Vogel-Fulcher (c), (d) fits of the “ T_f vs f ” curve respectively for T_{f1} and T_{f2} of $Bi_{1.9}Fe_{0.1}S_{0.15}Te_{2.85}$. 175

Figure 6.B.5: (a) Powder XRD pattern of $Bi_{1.9}Fe_{0.1}S_{0.15}Te_{2.85}$, (b) single crystal XRD and (c) powder XRD pattern of $Bi_{1.9}Fe_{0.1}Te_{2.85}$. 176

Figure 6.B.6: Temperature dependent angle resolved photoemission spectra taken at (a) 20K, (b) 150K, and (c) 260K with Synchrotron source of 95eV. 179

Figure 7.A.1: (a) Theoretical band structure of MoTeSe and (b) WTeSe with SOC at ambient conditions. 185

Figure 7.A.2: (a) Partial density of states (PDOS) of MoTeSe and (b) WTeSe at ambient pressure; inset: Total density of states (TDOS). 186

List of Figures

- Figure 7.A.3:** (a) PDOS and total DOS (inset) of MoTeSe at 3 GPa and (b) 10 GPa; (c) PDOS and total DOS (inset) of WTeSe at 3 GPa and (d) 10 GPa. 187
- Figure 7.A.4** (a) Theoretically obtained band structure of MoTeSe at 3 GPa and (c) 10 GPa; (b) WTeSe at 3 GPa and (d) 10 GPa. 188
- Figure 7.A.5:** (a) Evolution of lattice parameters a, b and c with pressure for MoTeSe and (c) WTeSe; (b) Volume as a function of pressure and the fitting of P-V data with 3rd order Birch-Murnaghan and Murnaghan equation of state for MoTeSe and (d) WTeSe. 189
- Figure 7.B.1:** Crystal structure of Sb₂Te₃. 195
- Figure 7.B.2:** Bandstructure of Sb₂Te₃ taking LDA approximation (a) without SOC; (b) with SOC. 197
- Figure 7.B.3:** Bandstructure of Sb₂Te₃ taking GGA approximation (a) at ambient pressure; (b) at 2GPa; (c) Partial and total DOS of Sb₂Te₃ at ambient pressure; (d) at 2 GPa. 198
- Figure 7.B.4:** Bandstructure of Sb₂Te₃ taking GGA approximation (a) at 7GPa pressure; (b) Comparison of lattice parameters with pressure. 199
- Figure 7.B.5:** (a) Volume as a function of pressure and the fitting of P-V data with 3rd order Birch-Murnaghan and Murnaghan equation of state for Sb₂Te₃; (b) c/a ratio as a function of pressure. 199
- Figure 7.B.6:** Electronic structure of the surface of Sb₂Te₃ along its (111) surface at (a) 0 pressure and (b) 7 GPa. The electronic states forming the Dirac cone have been marked with blue circle. 200

List of Tables

Table-3.1: The values of α extracted from HLN fitting.	91
Table 4.A.1: Comparison of experimental ETT and structural transitions (GPa) observed in various TIs.	104
Table 4.A.2: Lattice parameters and bulk modulus (obtained from BM EOS) for our experimental results of α -phase are compared with earlier published results.	105
Table 4.B.1: The lattice parameters and angles for different phases. Bulk modulus and its derivative are also depicted for initial phase.	123
Table 6.A.1: Parameters obtained from the ac susceptibility analysis for T_{f1} and T_{f2} .	160
Table 6.A.2: Parameters obtained from the ac susceptibility analysis for T_{f1} and T_{f2} .	160
Table 6.B.1: Parameters obtained from the Dynamic fitting analysis for T_{G2} .	175
Table 6.B.2: Parameters obtained from the V-F fitting analysis for T_{G2} .	175
Table 7.A.1: a comparative study of electronic and structural transition in MX_2 class of materials are given.	186
Table 7.B.1: Comparisons of ETT pressure in different TI materials.	198