

Contents

Acknowledgments	V
1 Introduction	1
2 Fundamentals of Topological Insulators	5
2.1 Introduction	5
2.2 Insulators with metallic boundary states	5
2.2.1 Integer quantum Hall effect	7
2.2.2 The Hall conductance as a topological invariant	8
2.2.3 Quantum spin Hall effect or time-reversal invariant 2D topological insulator	14
2.2.4 Construction of $\mathbb{Z}_2$ invariant for 2D topological insulators	19
2.2.5 Generalization to three-dimensions	29
2.2.6 Weak topological insulators	34
2.2.7 Experimental realizations of 3D topological insulators	36
3 Experimental Methods	41
3.1 Scanning tunneling microscopy	41
3.1.1 Tersoff-Hamann model	42
3.1.2 Scanning tunneling spectroscopy	44
3.1.3 STM and STS experiments	46
3.2 Angle-resolved photoemission spectroscopy	47
3.2.1 Spin-resolved ARPES	53
3.2.2 Experimental details: ARPES at the synchrotron	55
4 Identification of Tellurium based Phase-Change Materials as Strong Topological Insulators	59
4.1 Fundamentals of phase-change materials	60
4.2 Identification of topological insulator properties in crystalline Sb_2Te_3	65
4.2.1 STM and STS characterization of Sb_2Te_3	65
4.2.2 Spin-resolved ARPES measurements of Sb_2Te_3	74

4.3	Characterization of crystalline $\text{Ge}_2\text{Sb}_2\text{Te}_5$ in terms of topological insulator	89
4.3.1	Stacking order of $\text{Ge}_2\text{Sb}_2\text{Te}_5$ in the crystalline phase . . .	90
4.3.2	Preparation and characterization of metastable crystalline $\text{Ge}_2\text{Sb}_2\text{Te}_5$ samples	92
4.3.3	Evidence for topological band inversion in metastable crystalline $\text{Ge}_2\text{Sb}_2\text{Te}_5$ measured by ARPES	95
5	Weak Topological Insulator	105
5.1	General description of the first synthesized weak topological insulator $\text{Bi}_{14}\text{Rh}_3\text{I}_9$	105
5.2	Edge states at the dark side of the weak topological insulator $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ probed by STS	109
5.2.1	Identification of the atomic and electronic structure of the different layers in $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ by STM	109
5.2.2	Bias-dependent structural variations of the morphology of the 2D TI and spacer layer in $\text{Bi}_{14}\text{Rh}_3\text{I}_9$.	114
5.2.3	Probing the edge state at the step edge of the 2D TI layer in $\text{Bi}_{14}\text{Rh}_3\text{I}_9$	122
5.2.4	Evidence for the topological nature of the edge state in $\text{Bi}_{14}\text{Rh}_3\text{I}_9$	126
5.2.5	Absence of an edge state in the structural closely related but topologically trivial material $\text{Bi}_{13}\text{Pt}_3\text{I}_7$	134
5.2.6	Computational details	141
6	Summary	143
	Bibliography	145
	Publications	165