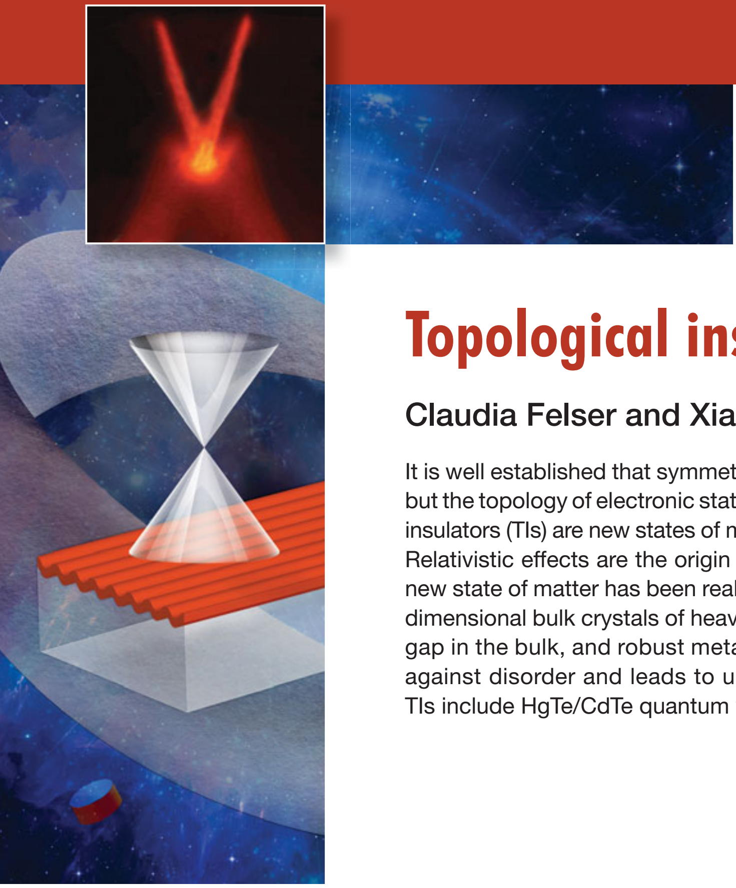

Topological insulators

Claudia Felser and Xiao-Liang Qi, Guest Editors

It is well established that symmetry has an important influence on the properties of materials, but the topology of electronic states might be an even more fundamental property. Topological insulators (TIs) are new states of matter based on the topology in the electronic band structure. Relativistic effects are the origin of the topologically non-trivial electronic structure, and the new state of matter has been realized in two-dimensional quantum well structures and three-dimensional bulk crystals of heavy elements and compounds. TI materials have an insulating gap in the bulk, and robust metallic edge/surface states on the boundary, which is robust against disorder and leads to unique spin and charge transport properties. Examples of TIs include HgTe/CdTe quantum wells, Bi-Sb-alloys, Bi_2Se_3, and half-Heusler compounds.

Introduction

Topological insulators (TIs), discovered in the past decade, represent a new state of matter. TI materials have an insulating gap in the bulk and robust metallic edge/surface states on the surface.[1–11] The topology for most insulators and semiconductors is trivial. Relativistic effects are the origin of the topologically non-trivial electronic structure, and as a consequence, most TIs contain heavy elements such as bismuth, platinum, or tellurium. TIs have been realized in both two-dimensional thin films and three-dimensional bulk crystals. In both two and three dimensions, the surface states of TIs are "helical," which means the spin of the surface state electron is locked in the direction of its velocity, as illustrated in **Figure 1**. As a consequence of this helical property, elastic backscattering of the surface state is completely suppressed as long as time-reversal symmetry is preserved. Due to the time-reversal symmetry, back-scattering processes with clockwise and counter-clockwise spin rotation always have the same amplitude and opposite sign, which thus intefere destructively and result in perfect transmission of electrons.[1] Additionally, this property guarantees the robustness of the surface states against disorder and leads to unique spin and charge transport properties of TIs. In particular, the edge state of two-dimensional TIs carries a unidirectional spin current, which is why the two-dimensional TI is also known as the quantum spin Hall (QSH) state.

The discovery of TIs has led to a paradigm shift in condensed matter physics on two levels: (1) TI is a new state of quantum matter that enables the development of new technologies. (2) The dissipationless transport of the surface states can enable low power electronics applications. Additionally, it is the first successful example of the predictive power of theory in material science.

Materials and their properties

Many different experimental techniques have been applied to study TI materials, including transport measurements, angle-resolved photo-emission spectroscopy (ARPES), scanning tunneling microscopy (STM), and optical conductivity. For three-dimensional TIs, ARPES allows for the most direct measurement of the dispersion of surface states, which can be used to determine the topological nature of the material. For two-dimensional TIs, the edge states have been studied in various transport experiments. As examples of the interesting physical properties of TIs, in **Figure 2** we show some representative experimental data on (a) the conductance of the two-dimensional QSH state in HgTe[12] and (b) three-dimensional Bi_2Te_3 and Bi_2Se_3 surface states observed in ARPES.[13,14]

New physical effects, such as the quantum anomalous Hall effect (QAHE),[15,16] topological magnetoelectric effect,[17,18] and topological surface superconductivity,[19] have been proposed for TIs, thus making TIs interesting candidate systems for

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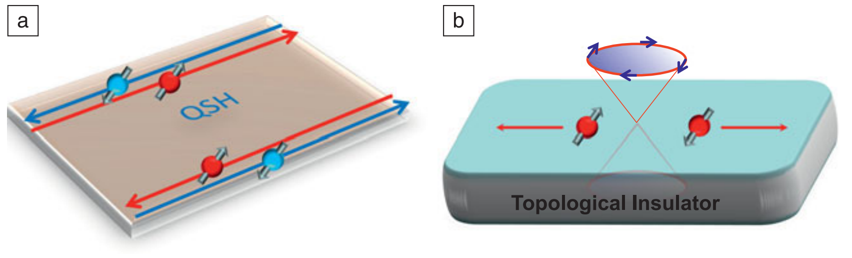

Figure 1. Schematic picture of the edge/surface states of (a) the two-dimensional quantum spin Hall state, and (b) three-dimensional topological insulator.

new spintronics devices and topological quantum computation. In particular, the QAHE (i.e., an integer quantized Hall effect without an external magnetic field) has recently been experimentally realized in magnetically doped TI thin films in the Bi_2Se_3 family.[20] This is a direct physical manifestation of the topological nature of the TI surface states. Figure 2c shows the Hall conductance as a function of magnetic field for the Cr-doped $Bi(Sb)_2Te(Se)_3$ thin film and the QAHE around zero external field.[20]

Research on TIs has recently become one of the most active new fields in condensed matter physics. Materials science efforts are essential for the realization of the physical effects and device concepts proposed for TIs, and for the discovery of new TI materials. The articles in this issue of *MRS Bulletin* aim to provide an overview of the field of TIs for materials scientists and to inspire new theoretical and experimental developments in this exciting field of research.

One fascinating aspect of TIs is that theory has been providing reliable guidance to materials discoveries.[21,22] Many TIs have first been predicted theoretically and have subsequently been realized experimentally. These include the two-dimensional TIs–HgTe quantum wells and InAs/GaSb quantum wells, and the three-dimensional TIs–Bi_xSb_{1-x}, Bi_2Se_3, Bi_2Te_3, Sb_2Te_3, $TlBiSe_2$, and $TlBiTe_2$.[4,12,13,19,23–29] Potential TI candidates can be preselected by chemical intuition and by using some simple criteria such as semiconductors containing heavy elements. Density functional theory calculations can be applied to predict whether a given material can be a TI. Several different criteria have been proposed for determining the topological nature of a band structure, including surface state calculations,[17,30] parity inversion counting at high symmetry points in the Brillouin zone,[4,19,22] and Wilson loop spectral flow.[31]

For systems with inversion symmetry, the Bloch states at the inversion symmetric momenta, such as (0,0,0) and (π,π,π), are inversion symmetric and have a definite parity. The parity inversion criteria then counts the parity of occupied states at these points, and looks for "band inversion" defined by the difference between the parity eigenvalues of states at different inversion symmetric momenta. Since this method only applies to inversion symmetric systems, other criteria have been proposed for more generic systems without inversion symmetry. Among them, the Wilson loop spectral flow method is an intuitive way of tracking the motion of bulk electrons. This method finds the center-of-mass position of "hybrid Wannier states," which are local in real space in one direction (e.g., x direction) and are plane waves in perpendicular directions. The dependence of the center-of-mass position in x to perpendicular momenta describes how bulk electrons move in a perpendicular electric field, and characterize the topological nature of the system. The article by Weng et al. in this issue reviews the prediction and exploration of TIs by the first-principles calculation approach. Different methods of calculating topological invariants are reviewed, with an emphasis on the Wilson loop approach. The authors also provide an overview of recent progress in TI-related materials, including quantum anomalous Hall insulators, large-gap QSH insulators, and correlated TI.

A large number of TIs have been proposed thus far, and many of them have been realized experimentally. **Table I**

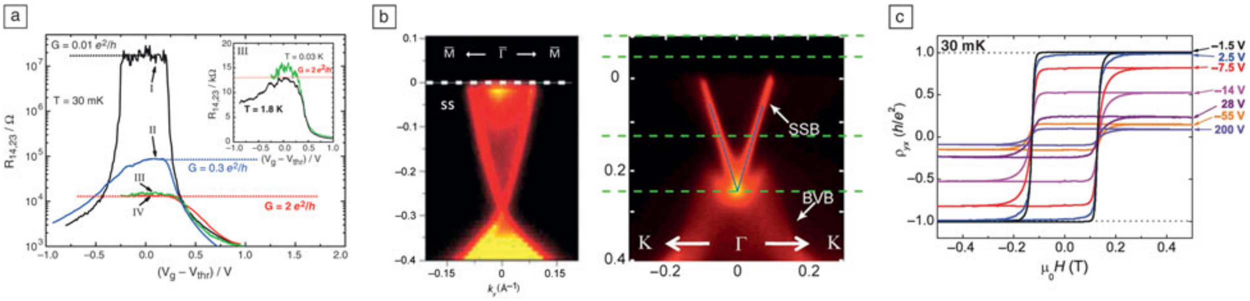

Figure 2. (a) Conductance of HgTe/CdTe quantum wells in the quantum spin Hall phase (II, III, IV) and in the trivial insulating phase (I).[12] (b) Angle-resolved photo-emission spectroscopy (ARPES) experiments showing the surface state dispersion of Bi_2Se_3 (left[13]) and Bi_2Te_3 (right[14]). (c) Hall conductance as a function of magnetic field for Cr-doped $Bi(Sb)_2Te(Se)_3$ thin film, showing the quantized anomalous Hall effect around zero external field.[20]

Table I. Proposed topological insulator materials grouped into several different material classes.[4,12,13,19,23–29]

HgTe-type	Bi_2Se_3-type	Honey Comb Lattice	Bismuth-Alloys	NaCl Structure	Oxides	Correlated Materials	Super-conductors
HgTe	Bi_2Se_3, Bi_2Te_3, and Sb_2Te3	Graphene	Bi-Sb	SnTe PbTe	Doped $BaBiO_3$	Iridates	$Cu_xBi_2Se_3$
Half-Heuslers such as LaPtBi	Bi_2Te_2Se	LiAuTe		PuTe AmN	Iridates	SmB_6	LaPtBi YPtBi LuPtBi
α-Sn, HgSe β-HgS	$(Bi_xSb_{1-x})_2Te_3$					YbPtBi	$TlBiSe_2$ $TlBiTe_2$
Chalco-pyrites	$TlBiSe_2$ and $TlBiTe_2$					Skutterudites	
AlSb/InAs/GaSb	$Bi_{14}Rh_3I_9$					PuTe, AmN	

lists various TI materials grouped into different families based on their structure, electronic structure, and bonding. The predicted materials cover nearly all areas of condensed matter physics. Among the proposed TIs, there is a large family of half-Heusler compounds, which are multifunctional materials combining properties such as superconductivity and magnetism with the topological band inversion.[32,33] Yan and de Visser's article in this issue provides an overview of half-Heusler TIs, including a summary of effective model description and physical properties. An interesting aspect of half-Heusler TIs is that several materials in this family become non-centrosymmetric superconductors at low temperature. The combination of topological band structure and non-centrosymmetric superconductivity may lead to another interesting topological phase—time-reversal invariant topological superconductors with the appearance of Majorana fermions.[19] Majorana fermions are fermionic particles that are expected to be their own antiparticles and are potential building blocks for quantum computation. The theoretical discussion about this possibility is also reviewed in the article by Yan and de Visser.

From the list of proposed materials in Table I and beyond, only a limited number have been synthesized, and an even smaller number of them have been proven to be TIs. The need for more high-quality materials in the form of single crystals, nanoparticles, thin films, and in devices is obvious. In the other two articles in this issue, two different growth methods for TIs are reviewed. The article by Chang et al. gives an overview of the current status of thin-film research for TIs with a special focus on time reversal symmetry breaking with ferromagnetic perturbation. The observation of the QAHE in Cr-doped selenides was a breakthrough experiment in 2013.[20] The authors compare the physics of different doped films of TIs and heterostructures of TIs with ferromagnetic insulators and outline the prospects for future studies.

The article by Hong et al. gives an overview of TI nanostructures. Compared to bulk materials, nanostructures have a higher surface-to-bulk ratio, which allows topological properties of the surface states to be observed more clearly. This article reviews the growth of physical properties of TI nanostructures, including $Bi_{2-x}Sb_xTe_{3-y}Se_y$ nanoribbons. An important physical property of the nanoribbon is the Aharonov-Bohm (AB) effect, which demonstrates the existence of quantum coherent surface states. In addition, the AB effect in this system also shows qualitative differences from that in other systems, such as carbon nanotubes and semiconductor nanowires, as a consequence of the unique spin dynamics of the topological surface states. Experimental results on the AB effect in TI nanoribbons and the corresponding theoretical analysis are reviewed in the article by Hong et al.

Conclusion

For room-temperature application of TIs in future electronic devices, there is still a need for new materials with large bandgaps. High-quality samples for transport measurements and devices with well-defined interfaces are a challenge for materials science as well. Furthermore, the class of correlated insulating oxides with elements from periods 5 and 6 and their electronic structures should be investigated systematically under the view point of potential topological effects. With this issue, we hope to stimulate further materials research.

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