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# New Horizons of Topological Material Science

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**Abstract**

**Since the proposals of spin Hall effect and topological insulators, many topological materials have been found, even among known materials, and they exhibit novel properties unique to topological materials. We explain recent developments on topological aspects of materials science, and discuss perspectives for future applications.**

## 1. Introduction

Topological materials have been attracting much interest in condensed matter physics. The first and well-known example of topological systems is the quantum Hall system [1]. When we apply a strong magnetic field onto a two-dimensional electron gas, the Hall conductivity is quantized and topological chiral edge states appear at the edges of the system. Nonetheless, because it requires a strong electric field, possibilities for its applications are limited.

Meanwhile, theoretical proposals of the spin Hall effect [2,3] have triggered new possibilities for topological systems [4]. Prior to these proposals, Hall effects and topological phases were thought to be possible only when the time-reversal symmetry is broken, i.e. when a magnetic field or magnetism is present in the system. In contrast, the spin Hall effect is realized in nonmagnetic metals and semiconductors, and the topological insulators are found in various narrow-gap semiconductors. In my presentation, we show recent developments in the field of topological materials, and discuss perspectives for future applications.

## 2. Berry curvature and spin Hall effect

Through the studies on Hall effect, it has been established that the equations of motion of electrons in a crystal have a term proportional to the Berry curvature. The equations of motion for electrons in a crystal are written as

$$\dot{\boldsymbol{x}} = \frac{1}{\hbar}\frac{\partial E_n(\boldsymbol{k})}{\partial \boldsymbol{k}} - \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}_n(\boldsymbol{k}), \qquad (1)$$

$$\dot{\boldsymbol{k}} = -e\boldsymbol{E}, \qquad (2)$$

where $\boldsymbol{x}$ is the position, $\boldsymbol{k}$ is the wavevector, $E_n$ is the electron energy in the $n$th band, and $\boldsymbol{E}$ is the electric field. $\boldsymbol{\Omega}_n(\boldsymbol{k})$ is the quantity called Berry curvature, defined as

$$\boldsymbol{\Omega}_n(\boldsymbol{k}) = i\left\langle \frac{\partial u_{nk}}{\partial \boldsymbol{k}} \right| \times \left| \frac{\partial u_{nk}}{\partial \boldsymbol{k}} \right\rangle. \qquad (3)$$

If we ignore the second term of Eq. (1), the equations become the well-known semiclassical equations of motion for electrons. The Berry curvature term comes from a multi-band effect, and it leads to the motion of electrons which is perpendicular to the electric field, i.e. the Hall effect.

The Hall effect occurs only when the time-reversal symmetry is broken, i.e. in the presence of magnetism or magnetic field. Meanwhile, one can apply the equations of motion (1)(2) to nonmagnetic systems, which leads to various types of Hall effects such as spin Hall effect [2,3]. Namely, in a material with spin-orbit coupling, the Berry curvature depends on spin directions, and it leads to the spin-dependent transverse velocity, i.e. spin current induced by the electric field (Fig. 1). This is expected for a broad range of metals and doped semiconductors with spin-orbit coupling. Indeed, it has been observed in various materials.

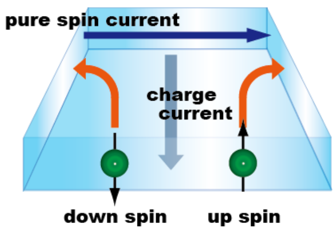


Fig. 1 Schematic figure of the spin Hall effect

## 3. Topological materials

By extending this idea to an insulator, one reaches a concept of topological insulators [4]. Schematic figures are shown in Fig.2 for (a) two-dimensional and (b) three-dimensional topological insulators. In these topological insulators, the bulk is insulating, while the edges/surfaces are metallic, carrying a pure spin current. Namely in equilibrium, up-spins and down-spins are persistently flowing along the edges/surfaces of the system.

These topological insulators are characterized by the $Z_2$ topological invariant, which can be calculated from the band structure calculation of the material. In addition to the topological insulator with the time-reversal symmetry, there are various topological insulators due to some spatial symmetries, called topological crystalline insulators. At present, many materials are known to belong to these types of topological materials.

These topological insulators show novel physical properties. For example, in the topological insulators, the edge can be regarded as a quantum wire supporting a pure spin current, and shows a quantized conductance, as has been observed in experiments. Another example is the quantum anomalous Hall effect [5]. By doping magnetic impurities into a topological insulator, one can realize a quantum Hall system due to ferromagnetism, without an external magnetic field. In such quantum anomalous Hall systems, the bulk is insulating and the edges are chiral, with their flow directions depend on the direction of the magnetization. This allows a switching of conduction paths by controlling the magnetic domains.

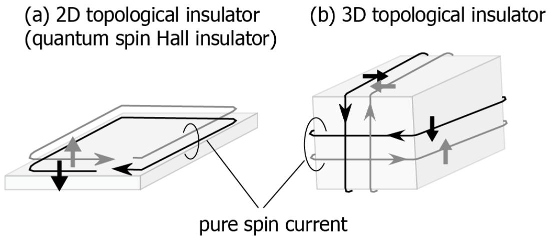


Fig. 2 Schematic figures of topological insulators for (a) 2D and (b) 3D.

## 4. Topological semimetals

Through the studies of topological insulators, proposals of topological band structures even in metals have been made. Such metals are called topological semimetals or topological metals. There are various types of topological semimetals, some of which are shown in Fig. 3. In Fig. 3, the dispersions of topological semimetals are shown schematically, with the vertical axis being the energy and the horizontal axes are the wavevector $\boldsymbol{k}$. In these topological semimetals, the valence bands and the conduction bands are degenerate at a point or a line in the $\boldsymbol{k}$ space, which is possible only when there is some reason from topology or symmetry in $\boldsymbol{k}$ space. For example, in the Weyl semimetal [6-8] (Fig.3(a)), the band gap closes at a point called a Weyl node, and this Weyl node is known as a monopole or an antimonopole for the Berry curvature. This topological nature protects the Weyl node from lifting its degeneracy.

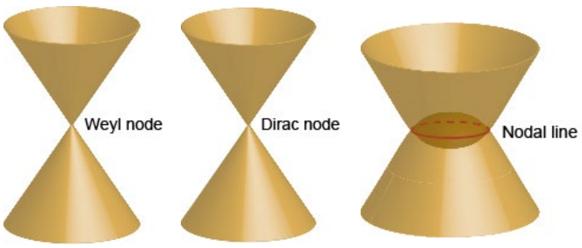


Fig. 3 Schematic band structures of topological semimetals. (a) Weyl semimetal, (b) Dirac semimetal and (c) nodal-line semimetal.

Because this degeneracy comes from topology and/or symmetry, one can control the band structure in a unique way, different from conventional materials. For example, in a superlattice with a topological semimetal with a normal insulator, various phases appear, and their phases are controlled in a unique way. For example, a switching behavior in a superlattice of the phase-change materials can be attributed to this topological nature of the materials [9].

## 4. Perspective for future applications

Unlike the quantum Hall system, which requires a strong magnetic field, the important aspect of the topological insulators and semimetals is that they can be realized without any external field, and there are many candidate materials to be used. Recently, a high-throughput search on topological materials has become available, based on materials databases, and now a large number of topological materials have been known. By a proper choice of materials and by introducing various types of external factors onto the materials, such as doping, alloying, change of system geometries such as thin films, quantum wells, and so on, one can have a broad range of controllability. Together with the novel physical properties of the system, topological materials promise various potential applications.

## 5. Conclusions

Topological materials turn out to be unexpectedly ubiquitous, including well known materials. Researches on topological materials have been opening a new frontier for materials science and for device applications. At present, the research is still in the fundamental level, but considering the rapid progress in this field in the past decade, we expect a yet more surprising progress in the coming decade.

## Acknowledgements


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