Solid State Communications 215-216 (2015) 54–62

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Transport properties of topological insulators: Band bending, bulk metal-to-insulator transition, and weak anti-localization

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ARTICLE INFO

Article history:
Received 23 July 2014
Accepted 17 October 2014
Communicated by Xincheng Xies
Available online 28 October 2014

Keywords:
A. Topological insulators
D. Transport properties

ABSTRACT

We reanalyze some of the critical transport experiments and provide a coherent understanding of the current generation of topological insulators (TIs). Currently TI transport studies abound with widely varying claims of the surface and bulk states, often times contradicting each other, and a proper understanding of TI transport properties is lacking. According to the simple criteria given by Mott and Ioffe–Regel, even the best TIs are not true insulators in the Mott sense, and at best, are weakly-insulating bad metals. However, band-bending effects contribute significantly to the TI transport properties including Shubnikov de-Haas oscillations, and we show that utilization of this band-bending effect can lead to a Mott insulating bulk state in the thin regime. In addition, by reconsidering previous results on the weak anti-localization (WAL) effect with additional new data, we correct a misunderstanding in the literature and generate a coherent picture of the WAL effect in TIs.

1. Introduction

Topological insulators (TIs) are a new class of matter that do not follow Landau's classification by spontaneously broken symmetry; rather they are distinguished only by considering which topological class they belong. The topological invariant is derived from the band structure properties of the bulk electrons, and in certain materials, sufficiently strong spin–orbit coupling causes the valence and conduction bands to invert, which results in the topological invariant to change and a topological surface states (TSS) to develop (see Refs. [1–4] and references therein). In the case of three dimensional (3D) TIs, such as Bi_2Se_3, and Bi_2Te_3, it was predicted and observed that the surface states span the bulk energy gap and have a linear Diraclike dispersion with chiral spin-momentum locking [5–7]. Unlike typical surface states in insulators and metals, the surface states in TIs have an odd number of Dirac points, which are protected by time-reversal symmetry against localization effects. However, it was soon realized that all the materials that have these Dirac-like TSS are in fact not true TIs; all the known materials suffer from significant charge defects that push the Fermi level (E_F) into either the conduction band (CB) or the valence band (VB), and therefore should be referred to not as TIs, but rather as topological conductors. This parallel channel complicates transport experiments because it is difficult to distinguish between effects from the TSS and those that originate from this bulk state.

Here we present a coherent picture for understanding transport measurements on the current generation of TIs. In Section 2 we develop and apply the simple Mott and the Ioffe–Regel criteria for metal-to-insulator transitions and show that the majority of the best TI samples are in fact still metallic in the bulk. In Section 3, we develop and discuss band-bending effects, which helps understand some of the widely varying data in the literature particularly focusing on Shubnikov de-Haas oscillations. Then, we show that the band-bending effect can help overcome the Mott limit and a truly bulk insulating state can develop in the thin regime. Finally, in Section 4 we discuss the various aspects of the weak anti-localization (WAL) effect and their thickness dependences in TIs. This is all done in the context of experimental data.

2. Bulk metal-to-insulator transition

A condition for a material to become topologically non-trivial is for certain energy bands to invert (other promising examples such as topological Kondo insulators have recently been predicted [8] with experiments in the initial phase [9–13]). Band inversion is most easily achieved in narrow gap semiconductors that are predicted to have non-inverted bands, and by incorporating realistic spin–orbit coupling the energy bands invert [7]. However, in real materials there are a finite number of thermodynamically

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http://dx.doi.org/10.1016/j.ssc.2014.10.021
0038-1098/

induced atomic vacancies and anti-site defects that occur and act as charge defects, which shifts E_F. Since the band gap is narrow, E_F is easily moved into the bulk energy bands, and the material becomes metallic in the bulk. To get a feeling for how the bulk E_F changes as a function of bulk charge defect density, N_{BD}, we have plotted $E_F=\hbar^2/(2m*)(3\pi^2N_{BD})^{2/3}$ in Fig. 1, where we assumed an isotropic Fermi surface with the effective mass given in terms of the electron mass to be $m* \approx 0.15m_e$, a typical value for Bi_2Se_3 and Bi_2Te_3 [14]. Here and for all the following discussions, unless explicitly specified, the temperature is assumed to be absolute zero, which is a valid assumption for the commonly measured transport properties of TIs. What can be seen from this is that E_F is pinned within a few meV of the conduction band minimum (or valence band maximum in p-type materials) when the carrier density drops below $\sim 10^{17}$–10^{18}/cm^3. E_F can only become unpinned from the conduction band minimum and fall into the band gap if a metal-to-insulator transition occurs with reduced carrier densities; these transitions can occur via two different processes, Mott transition and Ioffe–Regel criterion.

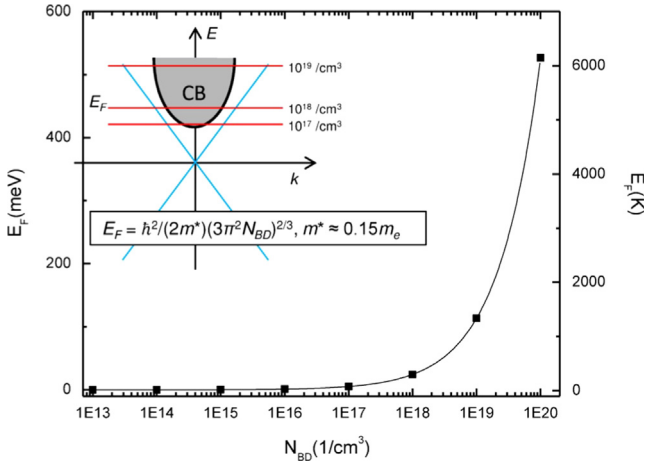

Fig. 1. The calculated Fermi energy, E_F, relative to the conduction band minimum, as a function of buk carrier density. Below a bulk defect density of $\sim 10^{17}$/cm^3, E_F is within a few meV of the conduction minumum. However, based on the Mott criterion, E_F will stay pinned in the bottom of the conduction band until the bulk defect density drops below the critical value of $\sim 3\times 10^{14}$/cm^3. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

When a dopant atom is embedded in an insulator, it forms a rescaled Coulomb potential, and this leads to hydrogenlike bound states, each with an effective Bohr radius given by $a_B=\varepsilon(m_e/m*)\times 0.5$ Å, where ε is the dielectric constant, m_e is the electron mass, $m*$ is the effective mass, and 0.5 Å is the free space Bohr radius. In a crystal, as the dopant density is increased, the mean separation of the dopant atoms decreases and eventually becomes comparable to the effective Bohr radius. When this happens, electrons that were bound to the dopant sites can become delocalized and freely move to neighboring sites, which gives rise to the insulator becoming a metal. The Mott criterion predicts that this happens when the dopant density passes the critical density given by $a_BN_M^{1/3} \approx 0.26$ (see Ref. [15]). Rearranging this, we then get the critical value to be $N_M \approx (m*/(\varepsilon m_e))^3 \times (1.4\times 10^{23}/\text{cm}^3) \approx 3\times 10^{14}/\text{cm}^3$ for both Bi_2Se_3 and Bi_2Te_3; this was found by using $\varepsilon \approx 110$ and $m* \approx 0.15m_e$ [14]. $N_M \approx 3\times 10^{14}/\text{cm}^3$ is extremely small compared to the corresponding numbers for common semiconductors such as Si where $N_M \approx 10^{18}/\text{cm}^3$. In fact, for Bi_2Se_3 the lowest dopant density achieved thus far is $\sim 10^{16}/\text{cm}^3$ (see Ref. [14]); it was found that these crystals were dominated by bulk carriers, which can be rationalized by considering the Mott criterion. In standard semiconductors such as Si, the bonding is very strong, and therefore a defect density of $\sim 10^{14}/\text{cm}^3$ is achievable in the cleanest materials. However in current TI materials, the bonding is much weaker, and therefore such a low defect density may be thermodynamically impossible to achieve either in intrinsic or in compensation-doped materials.

The Ioffe–Regel criterion explains how a metal transitions into an insulator with increased disorder and reduced carrier density. It states that the electrons in a metal become localized when the mean free path drops below the Fermi wave length [16]. In other words, the system remains metallic only if $k_Fl > 1$, where k_F is the Fermi wave vector and l is the mean free path, which can easily be calculated based on typical values measured by transport. Assuming a 3D isotropic Fermi surface $k_F=(3\pi^2N_{BD})^{1/3}$ and $l=(\hbar\mu/e)(3\pi^2N_{BD})^{1/3}$ where μ is the electron mobility, e is the electron

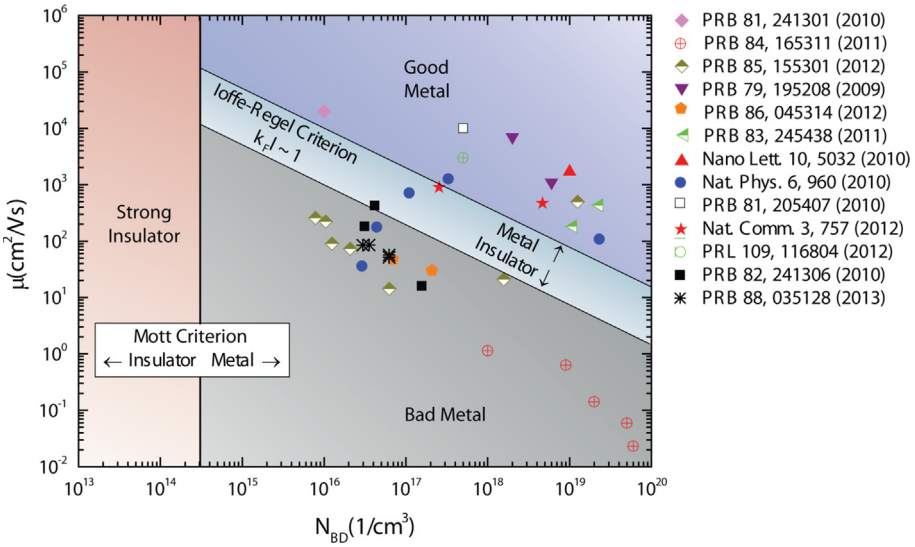

Fig. 2. The Mott and Ioffe–Regel criteria showing when a metal-to-insulator transition will occur based on the mobility and the bulk carrier density. The vertical line corresponds to a critical bulk defect density of $N_M \approx 3\times 10^{14}$/cm^3, while the diagonal lines correspond to $k_Fl \sim 0.3$–3: carrier densities and mobilities of representative Bi_2Se_3 and Bi_2Te_3 family of materials are shown together for comparison. What can be seen from this plot is that no known TI samples are truly an insulator in the Mott sense, and at best they are bad metals, exhibiting weakly insulating temperature dependence. Data are obtained from Refs. [14,18–29]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)