ARPES experiments on 3D topological insulators

Inna Vishik
Physics 250 (Special topics: spectroscopies of quantum materials)
UC Davis, Fall 2016
Outline

• Using ARPES to demonstrate that certain materials are 3D TIs
  • Surface states
  • Spin-momentum locking
  • Breaking TRS
• Fun with surface states
  • Surface/bulk coupling
  • 2-photon photoemission
  • Floquet-Bloch states
• Announcements
• Next lecture: ARPES experiments on other topological materials and Dirac materials including graphene, topological crystalline insulators, Dirac semimetals, Weyl semimetals
Materials

- $\text{Bi}_2\text{Te}_3$
- $\text{Bi}_2\text{Se}_3$
- $\text{Sb}_2\text{Te}_3$
- $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$

Materials history

I. INTRODUCTION

BISMUTH telluride recently has been of considerable interest, particularly as a thermoelectric material; however, the electrical and thermal properties of this material have not been established. The present paper describes the preparation of bismuth telluride of known composition and a study of the thermal conductivity and the electrical properties of both n- and p-type material.

This was found not to be the case. Whether the starting material contained an excess of Bi or an excess of Te the zone refined Bi₂Te₃ contained approximately 2×10⁹ excess holes.

By the technique described below the details of the phase diagram in the region of Bi₂Te₃ were clarified and also a series of single crystal samples of varying carrier concentration were produced for studies of the electrical and thermal properties.
Review: Quantum Hall "insulator" at B=0?

Look for large spin orbit coupling

- In a semi-classical approach we can consider electrons orbiting the nucleus.
- In the rest frame of the electron, the electric field turns into a magnetic field.

\[ B = -\frac{v \times E}{c^2} \propto r \times p = L \]

- And the SOC term is simply \( \mu_s \cdot B \). Momentum and the spin are perpendicular to one another.

This internal B-field from the spin-orbit coupling leads to the topological surface states. Because of the strong SOC, the spin \( S \) and the momentum \( k \) are locked perpendicularly.

- Originally proposed in 2D by Mele and Kane, 2005.
- The spin texture prevents back scattering.
Review: 3D Topological Insulator

- First generation of 3D topological insulators include: $\text{Bi}_{1-x}\text{Sb}_x$, $\text{Bi}_2\text{Se}_3$, $\text{Bi}_2\text{Te}_3$, $\text{Sb}_2\text{Te}_3$, $\text{Sb}$, etc...
- The “edge” of a 3D material is a 2D surface.
- Due to the spin texture, back scattering is still forbidden.
Disclaimer

Theory:
• This material is expected to be a topological insulator
• This will manifest in a certain electronic structure
  • Insulator in bulk
  • Dirac cone surface state
  • Spin texture

ARPES experiment:
• This material is a TI because theory says it is and we measure a consistent band structure
• Can measure
  • Band structure
  • Distinguish surface from bulk states
  • Spin texture
Expectations for ARPES spectra of 3D topological insulators

• Insulator in bulk

• Surface state
  • Odd number of them
  • Dirac-like dispersion
  • Spin-momentum locking
  • Difficult to destroy except by breaking time reversal symmetry
$0^{th}$ 3D Topological insulator: Bi$_{1-x}$Sb$_x$

Problem: too many surface states

1\textsuperscript{st} 3D Topological insulator: Bi$_2$Se$_3$

- Is this an insulator? (No, but we don’t care; Se vacancies in Bi$_2$Se$_3$ make it naturally n-type, but surface states still have expected properties)
- Concept: momentum distribution distribution curve (MDC) analysis (Intensity vs momentum at fixed energy)

Xia et al. Nat. Phys. 5 May 2009
Distinguishing surface from bulk states

Vary photon energy
- Surface bands **do not** disperse because they are strictly 2D
- Bulk bands **do** disperse because they have some 3D character
- Complication: matrix element effects can make surface state look brighter or dimmer at different photon energies

Xia *et al.* Nat. Phys. 5 May 2009
Fermi surface

Xia et al. Nat. Phys. 5 May 2009
2nd 3D topological insulator: Bi$_2$Te$_3$
Distinguishing surface from bulk in Bi$_2$Te$_3$

Similarities to Bi2Se3
- One dirac cone surface state per BZ
- Naturally n-type

Differences
- Star-shaped FS for surface state
- More pronounced dispersion for bulk state

Chen et al. Science 325 July 2009
Tuning doping: \((\text{Bi}_{1-\delta}\text{Sn}_\delta)_2\text{Te}_3\)

Same surface state, whether bulk is really insulating or not

Chen et al. Science 325 July 2009
Spin texture via spin ARPES

How can we measure electron spin in photoemission experiments?

<table>
<thead>
<tr>
<th>Method</th>
<th>Interaction</th>
<th>Operation voltage</th>
<th>$S_{\text{eff}}$</th>
<th>Figure of merit</th>
<th>Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mott</td>
<td>Spin-orbit</td>
<td>20–100 kV</td>
<td>0.1–0.2</td>
<td>1–5 × 10^{-4}</td>
<td>Au thin film</td>
</tr>
<tr>
<td>SPLEED</td>
<td>Spin-orbit</td>
<td>150 V</td>
<td>0.2–0.3</td>
<td>1–2 × 10^{-4}</td>
<td>W single crystal</td>
</tr>
<tr>
<td>Diffuse scattering</td>
<td>Spin-orbit</td>
<td>150 V</td>
<td>~0.2</td>
<td>~1 × 10^{-4}</td>
<td>Au thin film</td>
</tr>
<tr>
<td>VLEED</td>
<td>Spin-exchange</td>
<td>6–10 V</td>
<td>0.3–0.4</td>
<td>~10^{-2}</td>
<td>Fe single crystal</td>
</tr>
</tbody>
</table>

Mott Detectors

- Spin-orbit coupling (SOC): positively charged nucleus provides effective B-field in rest frame of electron:
  \[ B = -\frac{v}{c} \times E = -\frac{Ze}{r^3} v \times r = \frac{Ze}{mcr^3} L \]
- Magnetic moment of electron:
  \[ \mu_e = -\frac{g_s e}{2Mc} S \]
- Interaction between electron and effective B field of nucleus:
  \[ \nu_{LS} = -\mu_e \cdot B = \frac{Ze^2}{2m^2c^2r^3} L \cdot S \]
- Scattering cross section has angular asymmetry

Spin texture via spin ARPES

What is the expected ‘spin texture’ for an ordinary metal?
- Without spin-orbit coupling?
- With spin-orbit coupling?

Spin texture via circular dichroism

1. Measure ARPES spectrum with left-circularly polarized (LCP) light
2. Measure ARPES spectrum with right-circularly polarized (RCP) light
3. $\Delta I(E, k_x, k_y) = I_{LCP} - I_{RCP}$
Destroying the surface state

- Surface state is topologically protected: should be impervious to impurities
- Surface state is protected by time reversal symmetry: should be vulnerable to magnetic field or magnetic impurities

Summary part 1

• \( \text{Bi}_2\text{Se}_3, \text{Bi}_2\text{Te}_3 \), and related materials are the ‘hydrogen atoms’ of topological insulators

• Lots of circumstantial evidence that these materials are likely 3D Tis
  • Dirac-like surface state at TRIM
  • Surface state has spin texture (spin-momentum locking)
  • Surface states are robust, except when they are subjected to magnetic impurities

• Next: fun with Tis
  • Creative experiments which exploit surface states to demonstrate new physics or experimental technology, without necessarily caring about their topological nature
Vocabulary

ARPESable: materials which easily yield good ARPES spectra

Why is Bi$_2$Se$_3$ so ARPESable?
One class of experiment with ultrafast lasers: pump-probe experiments

- Pump:
  - Time: 100 fs
  - Intensity: 1 nJ

- Probe:
  - Electronic property
  - Time delay

Diagram shows the relationship between pump and probe over time.
Pump-probe experiments

The pump
- Purpose (depends on specific experiment)
  - Create specific excitation
  - Whack the electronic system on a timescale faster than lattice response
  - Cause destruction
- Frequency (depends on specific experiment)
  - 1.5 eV (straight out of the Ti-Sapph laser)
  - Mid-IR (70-500 meV—relevant to excitations in solids)

The probe
- Ascertains system’s response as a function of time delay from pump
- Defines what experiment you are doing
  - Optics (probe measures change in reflectivity or absorption)
  - THz (measures changes in optical conductivity at low frequencies)
  - ARPES (measures changes in band structure)
  - Many others
2 photon photoemission (2PPE) as a substitute for inverse photoemission

<table>
<thead>
<tr>
<th>Photoemission</th>
<th>Photon in, electron out</th>
<th>Measure <strong>occupied</strong> electronic states</th>
<th>Sub-meV resolution common</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inverse photoemission</td>
<td>Electron in, photon out</td>
<td>Measure <strong>unoccupied</strong> electronic states</td>
<td>~500 meV resolution</td>
</tr>
</tbody>
</table>

Use time-resolved ARPES to measure unoccupied states
- Pulse 1 (pump): make excitation into unoccupied state
- Pulse 2 (probe): perform photoemission out of pump-populated unoccupied state
- Time resolution is not very important, but light **intensity** is because this is 2\textsuperscript{nd} order process
2 PPE experiments in Bi$_2$Se$_3$

- 1.5 eV pump, 5.98 eV probe, $\Delta t \sim 100\, fs$
- 2$^{nd}$ surface state observed above $E_F$!
- Applicable to many different materials

Sobota et al. PRL 111, 136802 (2013)
Surface-bulk coupling in Bi2Se3

- 1.5 eV pump, 6 eV probe
- Pump deposits energy into electrons, effectively giving them higher temperature than surrounding lattice
- In ordinary metals: electron thermalization with lattice set by e-ph coupling
- In metallic surface state: hot electrons in surface state can cool down faster by thermalizing with bulk bands first

Wang et al. PRL 109, 127401 (2012)
Floquet-Bloch states

• Spatially periodic:

\[ H(r + R) = H(r) \]

\[ \Psi_{nk}(r) = e^{ik \cdot r} u_{nk}(r) \]

\[ u_{nk}(r + R) = u_{nk}(r) \]

\[ k \text{ and } k + nG \]

\[ (G = 2\pi/R) \]

• Temporally periodic

\[ H(t + T) = H(t) \]

\[ \Psi_\alpha(t) = e^{-\frac{i}{\hbar} \epsilon_\alpha (t-t_0)} \phi_\alpha(t) \]

\[ \phi_\alpha(t) = \phi_\alpha(t + T) \]

\[ \epsilon_\alpha \text{ and } \epsilon_\alpha + n\hbar\omega \]

\[ (\omega = 2\pi/T) \]

If you have both spatially and temporally periodic Hamiltonian, Eigenvalues are periodic both in \( k \) and \( E \)! \( \rightarrow \) Floquet-Bloch states!
Creating new states of matter with light

- Use mid-IR pump with energy **smaller** than band gap of Bi2Se3
- Use oscillating electric field of pump to create floquet-bloch state
- Photoinduced gaps at band crossings
- Circularly polarized light can open gap at Dirac point!

Wang et al. Science **342** 514 (2013)
Opening gaps with light!

Wang et al. Science 342 514 (2013)
Conclusions part 2

• $\text{Bi}_2\text{Se}_3$ and related compounds are the type 1a supernova of time-resolved ARPES
  • Measurement of unoccupied band structure
  • Surface-bulk coupling
  • Floquet-Bloch states
Additional (light) reading