ARPES experiments on 3D topological insulators

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Physics 250 (Special topics: spectroscopies of quantum materials)

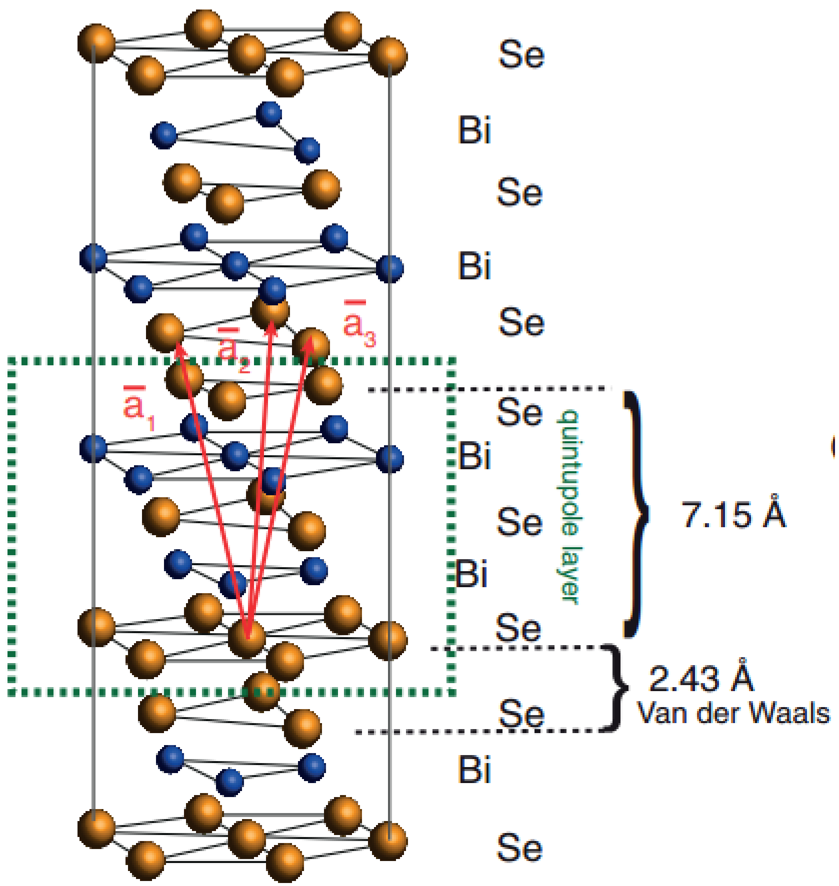
UC Davis, Fall 2016

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

- Bi_2Te_3
- Bi_2Se_3
- Sb_2Te_3
- $Bi_{2-x}Sb_xTe_{3-y}Se_y$



Bianchi *et al.* Semicond. Sci. Technol. **27** 124001 (2012)

Materials history

PHYSICAL REVIEW VOLUME 108, NUMBER 5 DECEMBER 1, 1957

Electrical and Thermal Properties of Bi_2Te_3

C. B. SATTERTHWAITE AND R. W. URE, JR.
Westinghouse Research Laboratories, Pittsburgh, Pennsylvania

(Received August 15, 1957)

Samples of both *n*-type and *p*-type Bi_2Te_3 containing from 3×10^{17} to 5×10^{19} extrinsic carriers were prepared and the phase diagram in the region about Bi_2Te_3 has been clarified. The Hall mobility parallel to the cleavage planes varies as $T^{-1.5}$ for holes and $T^{-2.7}$ for electrons. Room temperature values are $\mu_p=420$ cm² v⁻¹ sec⁻¹ and $\mu_n=270$ cm² v⁻¹ sec⁻¹. The energy gap is $E_g=0.20$ electron volts. From thermal conductivity measurements over the temperature range from 77°K to 380°K the lattice conductivity was found to be $\kappa_L=5.10\times10^{-2}/T$ watt-deg⁻¹ cm⁻¹. The sharp rise in the thermal conductivity in the vicinity of room temperature was attributed to transport of energy by ambipolar diffusion of electrons and holes.

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 Bi_2Te_3 contained approximately 2×10^{19} excess holes.

By the technique described below the details of the phase diagram in the region of Bi_2Te_3 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

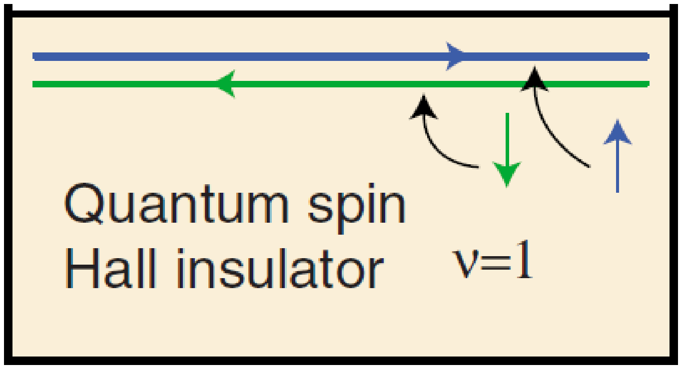
- In a semi-classical approach we can consider electrons orbiting the nucleus.
- In the rest frame of the electron, the electric field turns into a magnetic field.

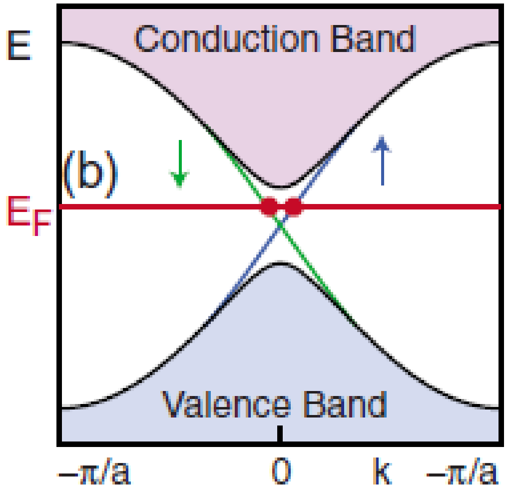
$$\boldsymbol{B} = -\frac{\boldsymbol{v} \times \boldsymbol{E}}{c^2} \propto \boldsymbol{r} \times \boldsymbol{p} = \boldsymbol{L}$$

- And the SOC term is simply $\boldsymbol{\mu_s} \cdot \boldsymbol{B}$ **.** *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.

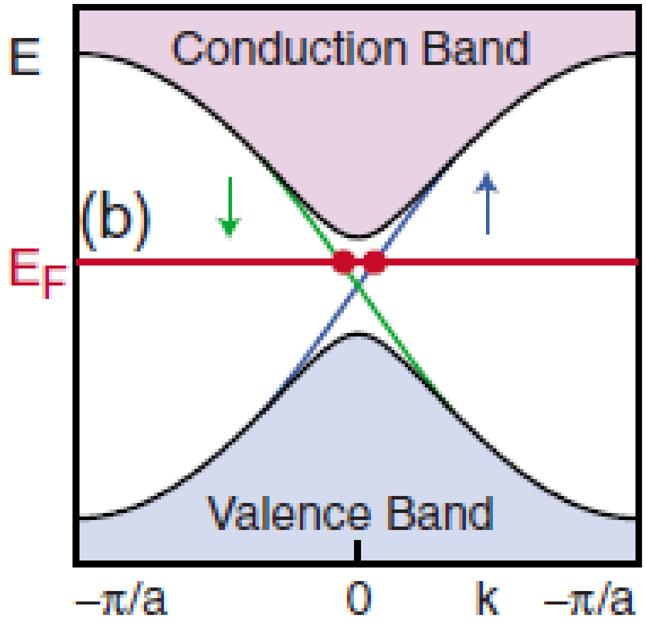
- Originally proposed in 2D by Mele and Kane, 2005.
- The spin texture prevents back scattering.

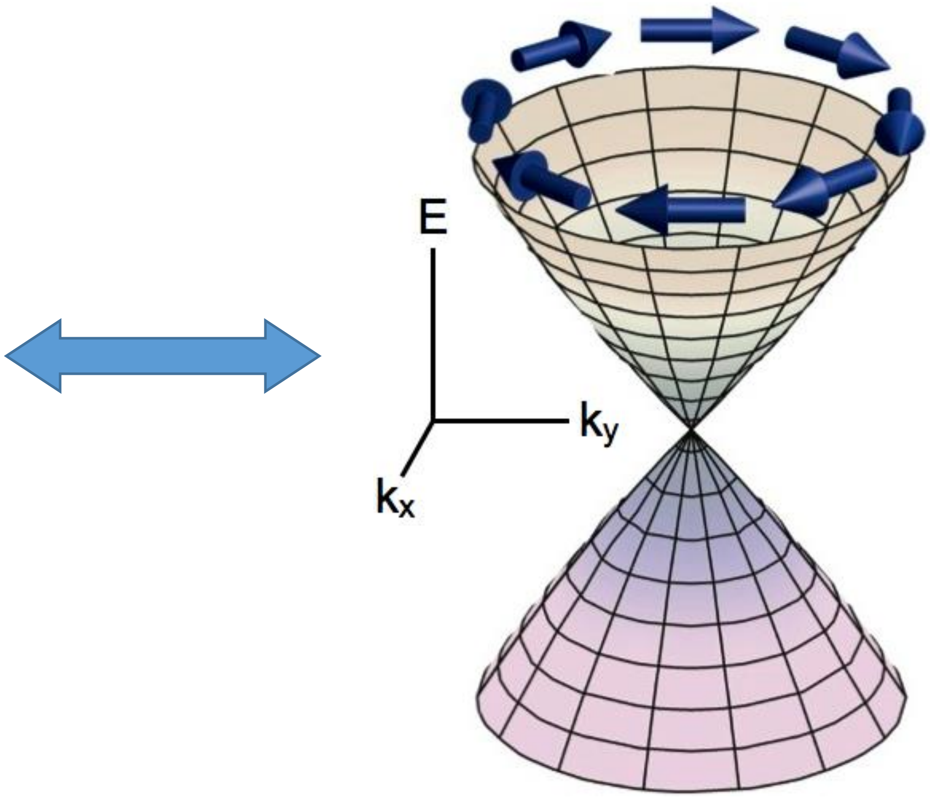




Review: 3D Topological Insulator

- First generation of 3D topological insulators include: $Bi_{1-x}Sb_x$, Bi_2Se_3, Bi_2Te_3, Sb_2Te_3, 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

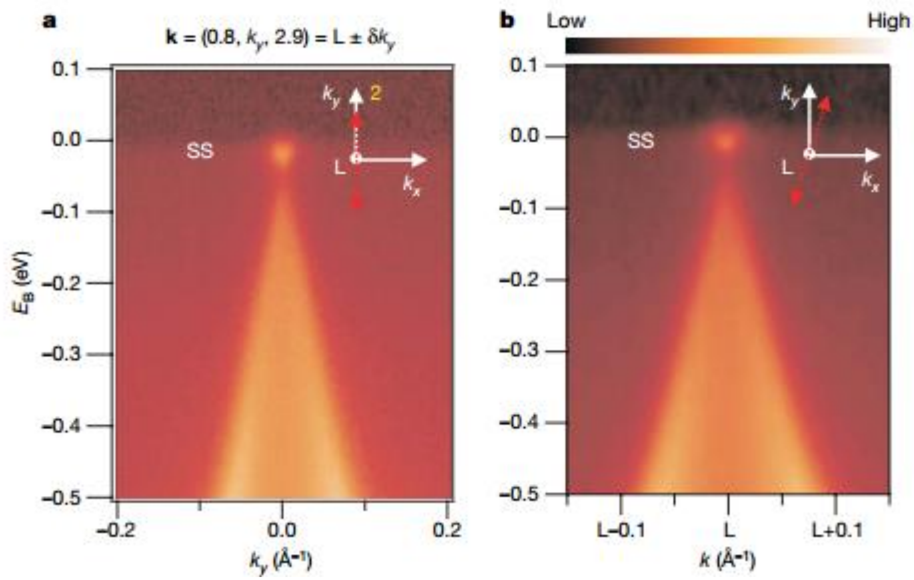
ARPES experiment:

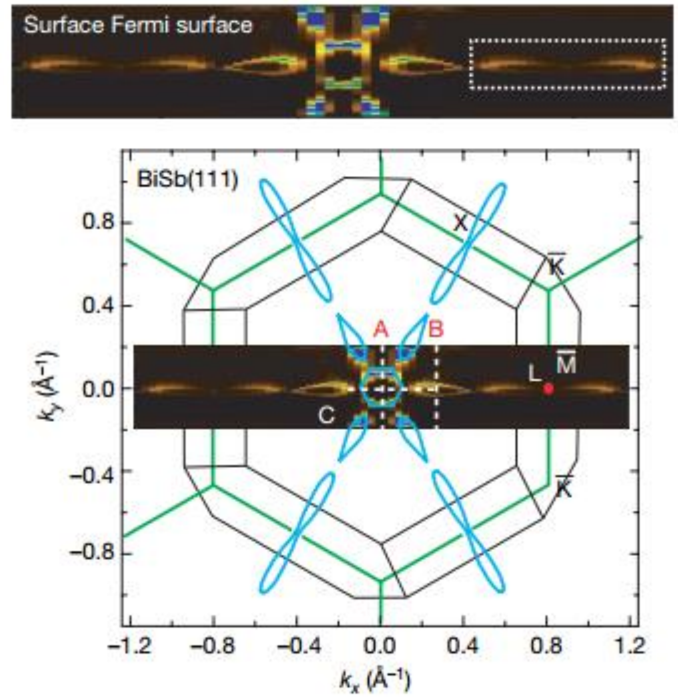
- This material is a TI because theory says it is and we measure a consistent band structure
- Can measure
    - Band structure
    - Distinguish surface from bulk states
    - Spin texture

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: $Bi_{1-x}Sb_x$

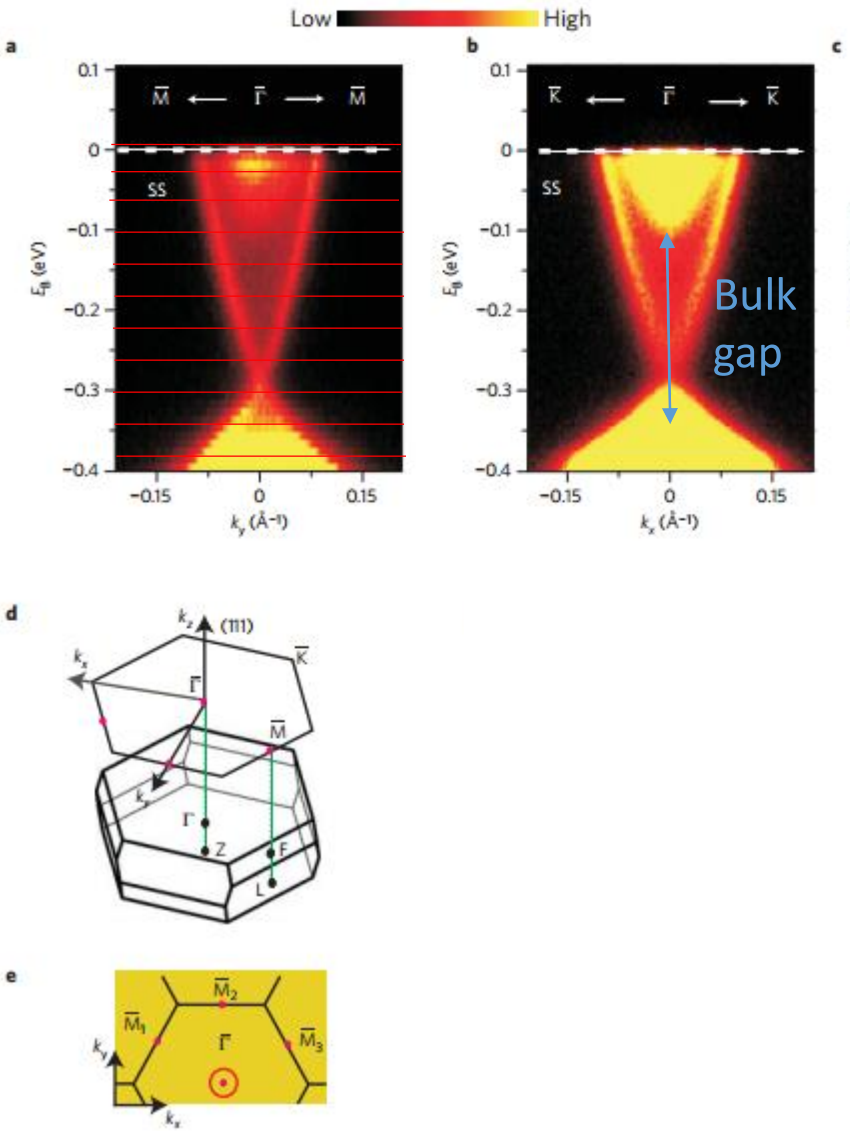




Problem: too many surface states

Hsieh *et al*. Nature **452** (2008)

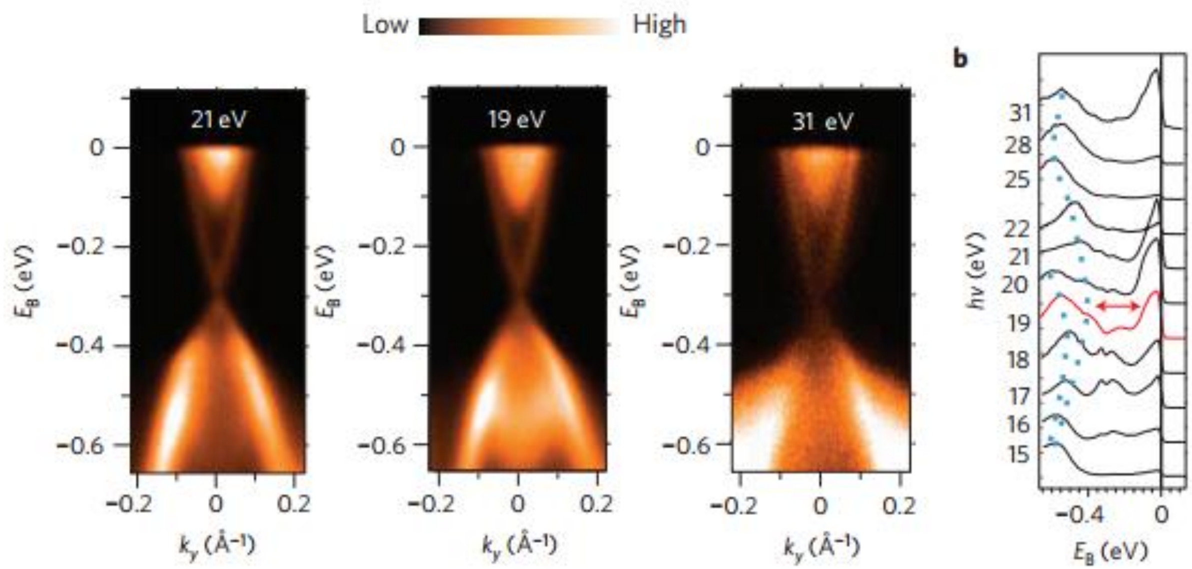
1st 3D Topological insulator: Bi_2Se_3



- Is this an insulator?
  (No, but we don't care; Se vacancies in Bi2Se3 make it naturally n-type, but surface states still have expected properties)
- Concept: momentum distribution curve (MDC) analysis
  (Intensity vs momentum at fixed energy)

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

Distinguishing surface from bulk states

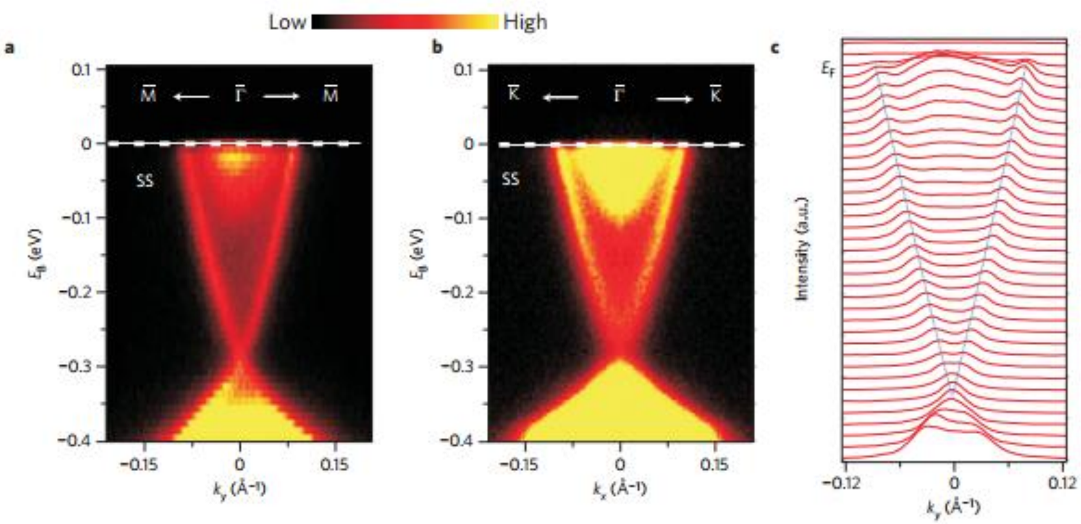


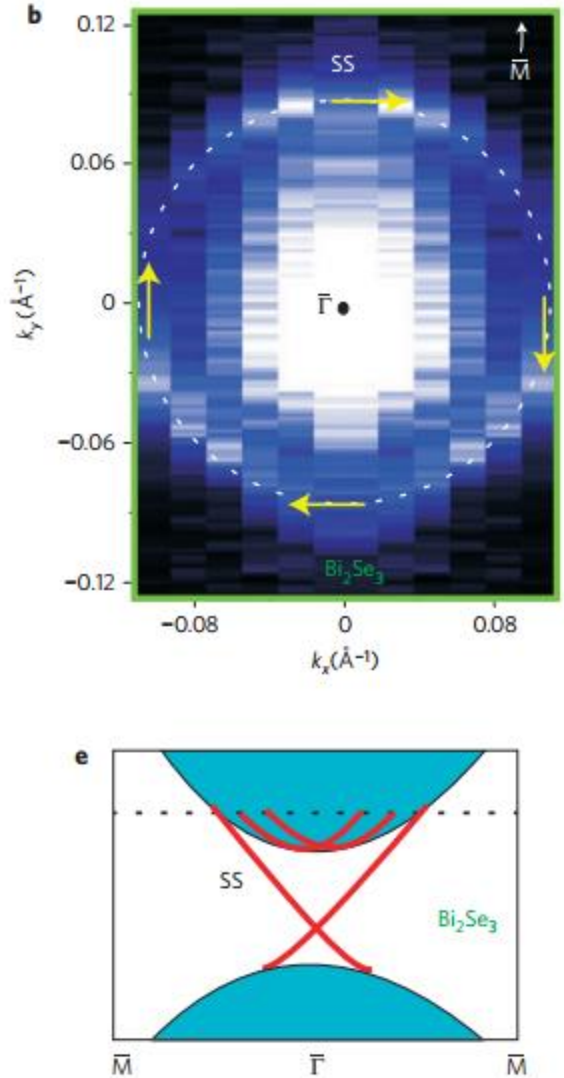
Vary photon energy

- 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

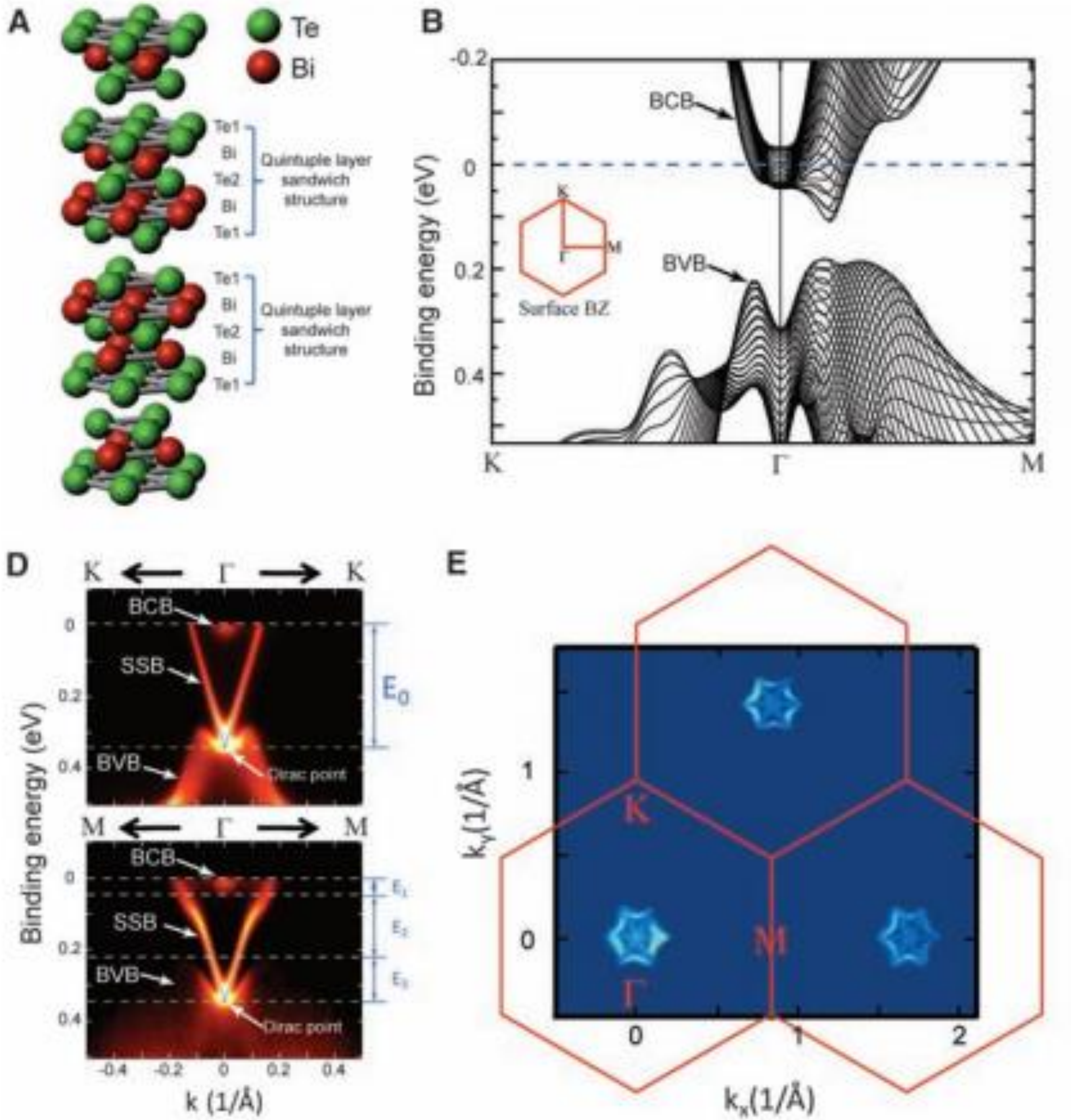
Fermi surface





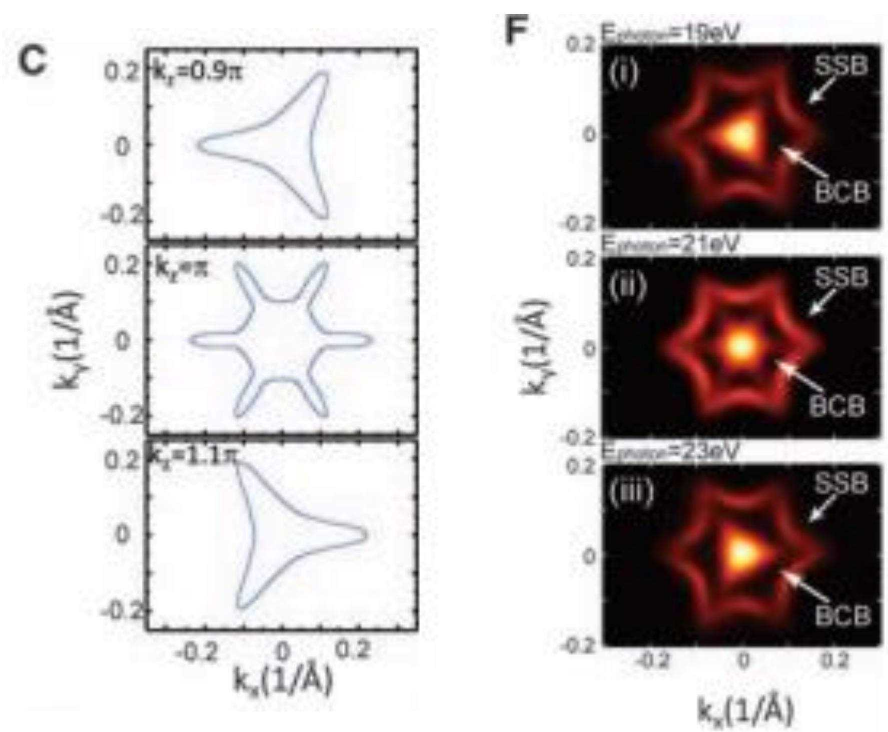
Xia *et al.* Nat. Phys. **5** May 2009

2^{nd} 3D topological insulator: Bi_2Te_3



Chen *et al.* Science **325** July 2009

Distinguishing surface from bulk in Bi_2Te_3



Similarities to Bi2Se3

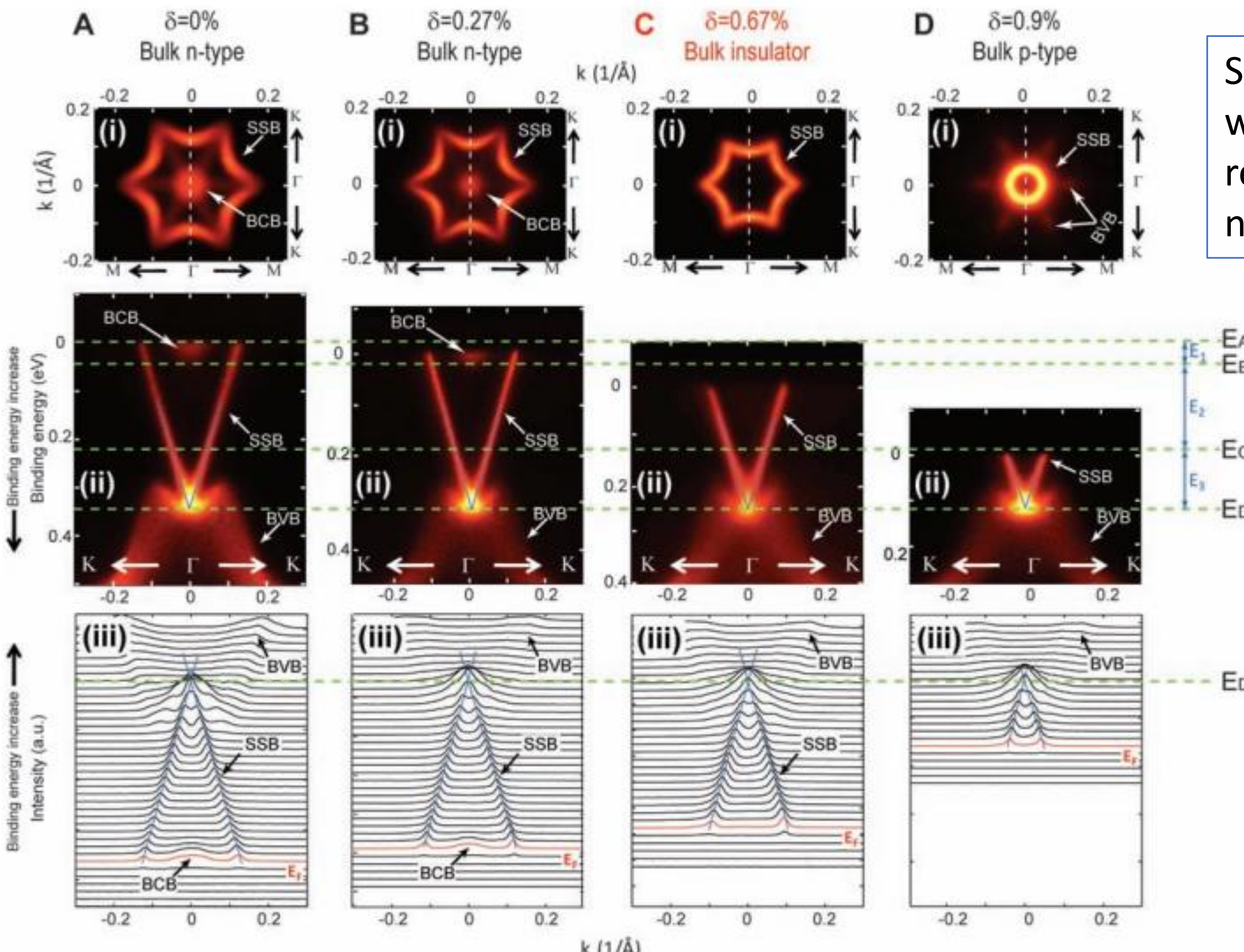
- One dirac cone surface state per BZ
- Naturally n-type

Differences

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

Chen *et al.* Science **325** July 2009

Tuning doping: $(Bi_{1-\delta}Sn_{\delta})_2Te_3$



Same surface state, whether bulk is really insulating or not

Chen *et al.* Science **325** July 2009

Spin texture via spin ARPES

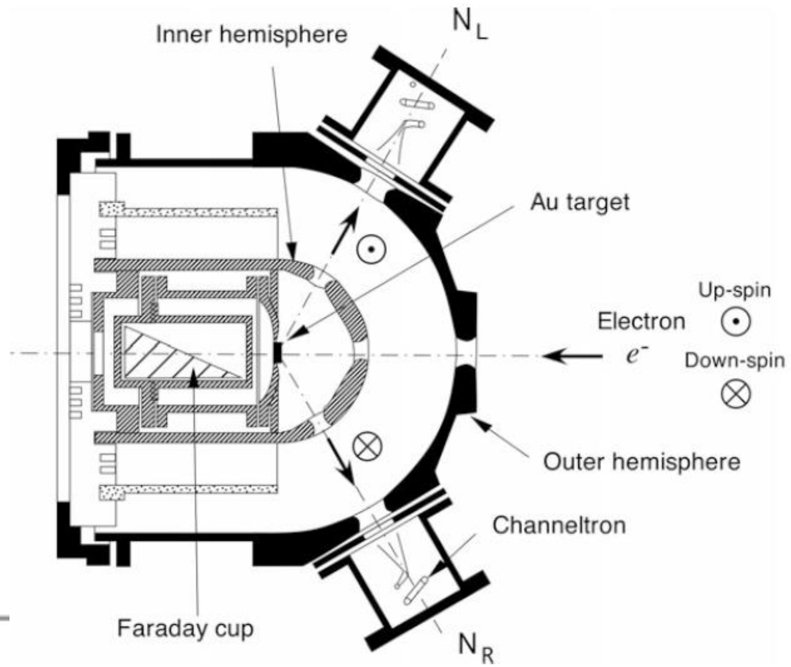
How can we measure electron spin in photoemission experiments?

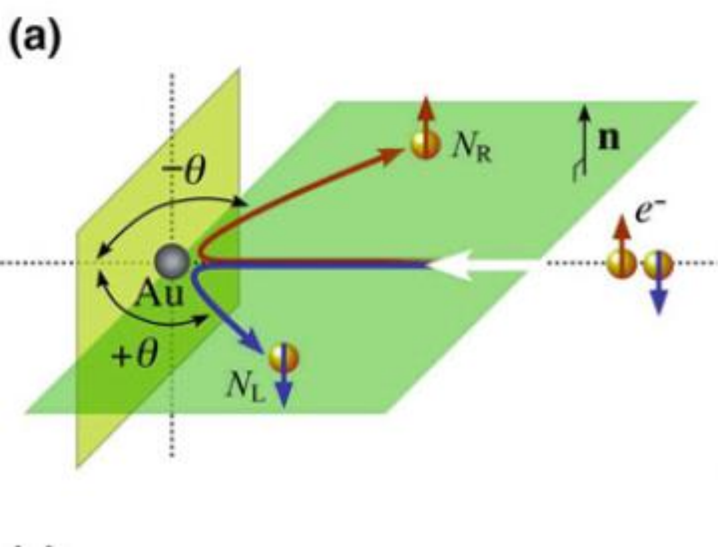
Method	Interaction	Operation voltage	S_{eff}	Figure of merit	Target
Mott	Spin-orbit	20–100 kV	0.1–0.2	$1\text{–}5 \times 10^{-4}$	Au thin film
SPLEED	Spin-orbit	150 V	0.2–0.3	$1\text{–}2 \times 10^{-4}$	W single crystal
Diffuse scattering	Spin-orbit	150 V	~0.2	$\sim 1 \times 10^{-4}$	Au thin film
VLEED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

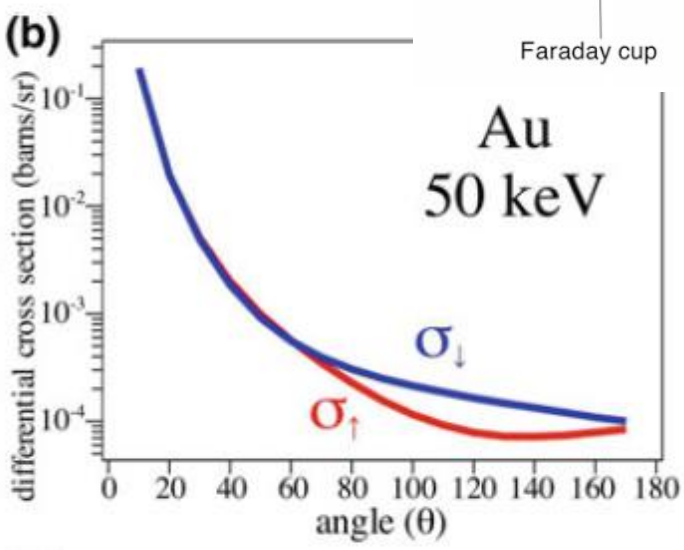
A. Takayama, *High-resolution spin-resolved photoemission spectrometer and the Rashba effect in Bismuth thin films (2015)*

Mott Detectors

- Spin-orbit coupling (SOC): positively charged nucleus provides effective **B**-field in rest frame of electron:
$$\boldsymbol{B} = -\frac{1}{c}\boldsymbol{v} \times \boldsymbol{E} = -\frac{1}{c}\frac{Ze}{r^3}\boldsymbol{v} \times \boldsymbol{r} = \frac{Ze}{mcr^3}\boldsymbol{L}$$
- Magnetic moment of electron:
$$\mu_e = -\frac{g_s e}{2mc}\boldsymbol{S}$$
- Interaction between electron and effective B field of nucleus:
$$v_{LS} = -\mu_e \cdot \boldsymbol{B} = \frac{\mathrm{Ze}^2}{2\mathrm{m}^2\mathrm{c}^2\mathrm{r}^3}\mathrm{L} \cdot \boldsymbol{S}$$
- Scattering cross section has angular asymmetry

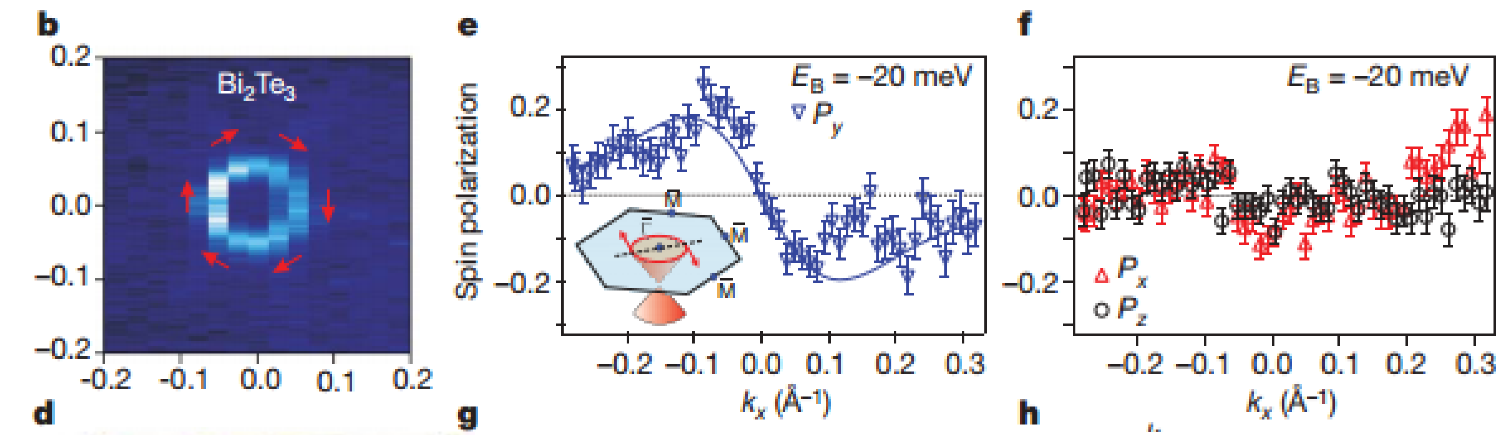


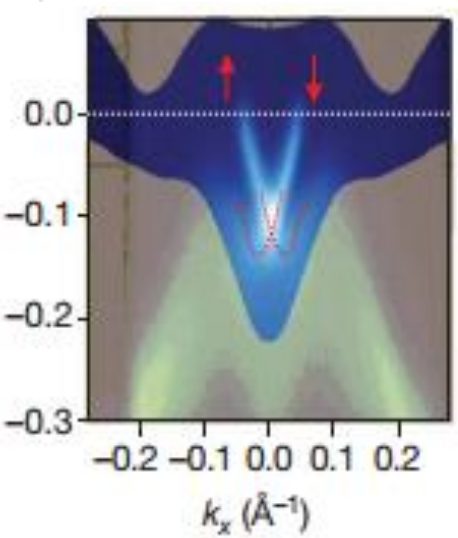




A. Takayama, *High-resolution spin-resolved photoemission spectrometer and the Rashba effect in Bismuth thin films (2015)*

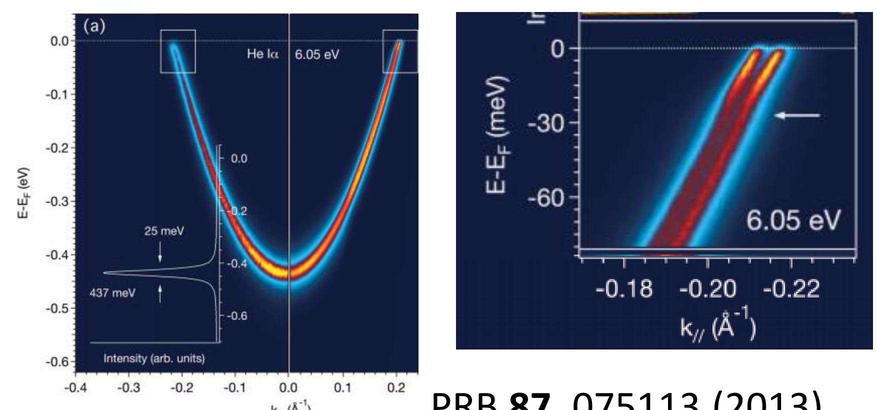
Spin texture via spin ARPES





What is the expected ‘spin texture’ for an ordinary metal?

- Without spin-orbit coupling?
- With spin-orbit coupling?

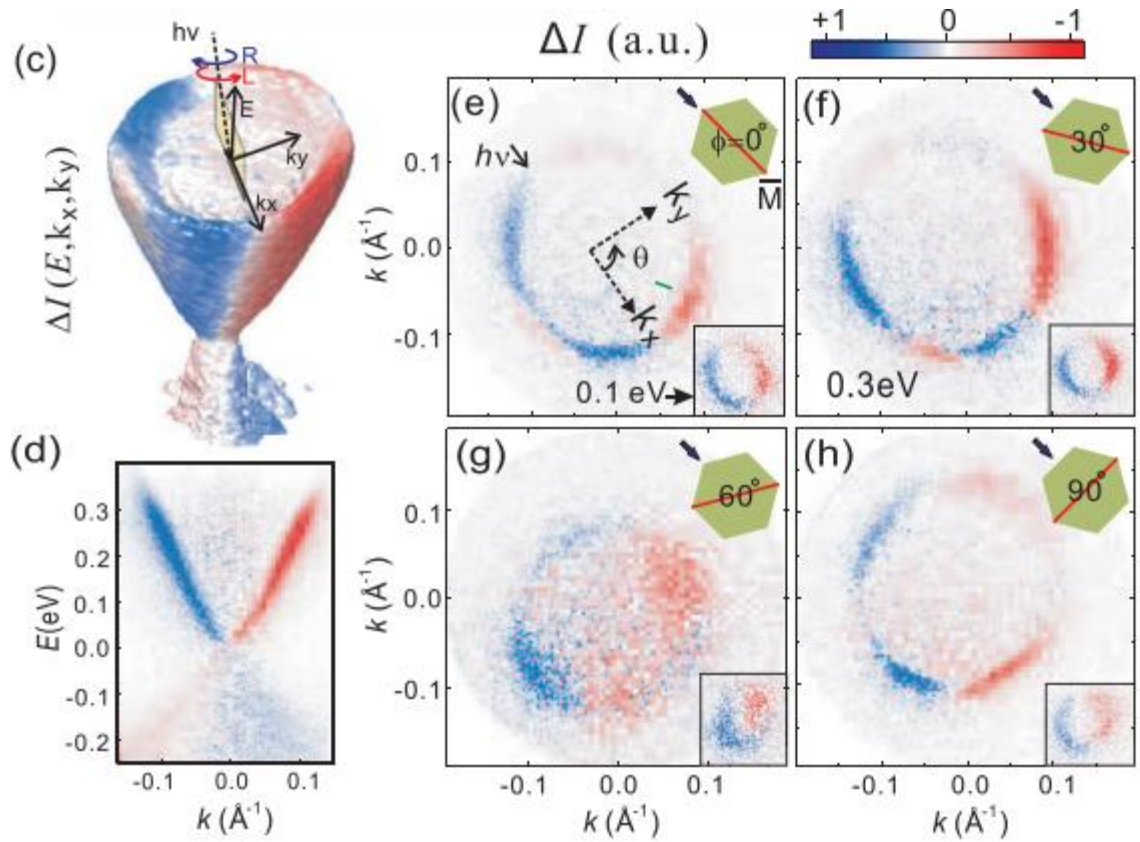


Hsieh *et al.* Nature **460** (2009)

PRB **87**, 075113 (2013)

Spin texture via circular dichroism

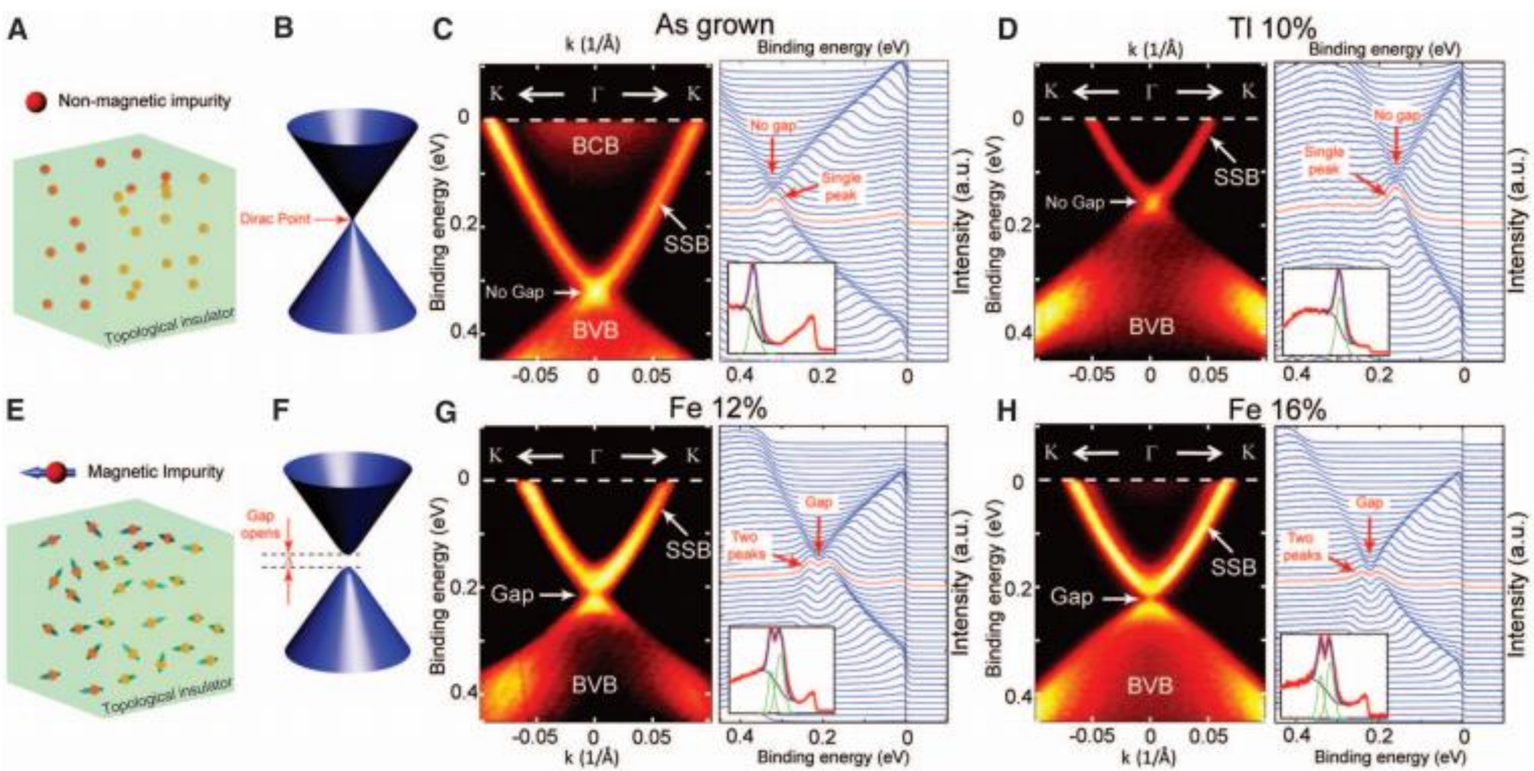
1. Measure ARPES spectrum with left-circularly polarized (LCP) light
2. Measure ARPES spectrum with right-circularly polarized (RCP) light
3. $\Delta I(E, k_x, k_y) = I_{LCP} - I_{RCP}$



Wang *et al.* PRL **107**, 207602 (2011)

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



Chen *et al.* Science **329** (2010)

Summary part 1

- Bi_2Se_3, Bi_2Te_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

ELSEVIER

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SCIENCE DIRECT

Journal of Physics and Chemistry of Solids 67 (2006) 201–207

JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS

www.elsevier.com/locate/jpcs

Life of the nodal quasiparticles in Bi-2212 as seen by ARPES

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Abstract

While the pronounced doping dependence of the quasiparticle spectral weight in the antinodal region of the superconducting cuprates, as seen by ARPES, unambiguously points to the magnetic origin of the strong electron–boson coupling there, the nature of the electron scattering in the nodal direction remained unclear. Here we present a short review of our recent detailed investigations of the nodal direction of Bi-2212. Our findings prove the existence of well defined quasiparticles even in the pseudogap state and show that the essential part of the quasiparticle scattering rate, which appears on top of Auger-like electron–electron interaction, also implies a magnetic origin.

Keywords: A. Superconductors; C. Photoelectron spectroscopy; D. Electronic structure; D. Superconductivity

PACS: 74.25.Jb; 74.72.Hs; 79.60.−i; 71.15.Mb

1. ARPES view

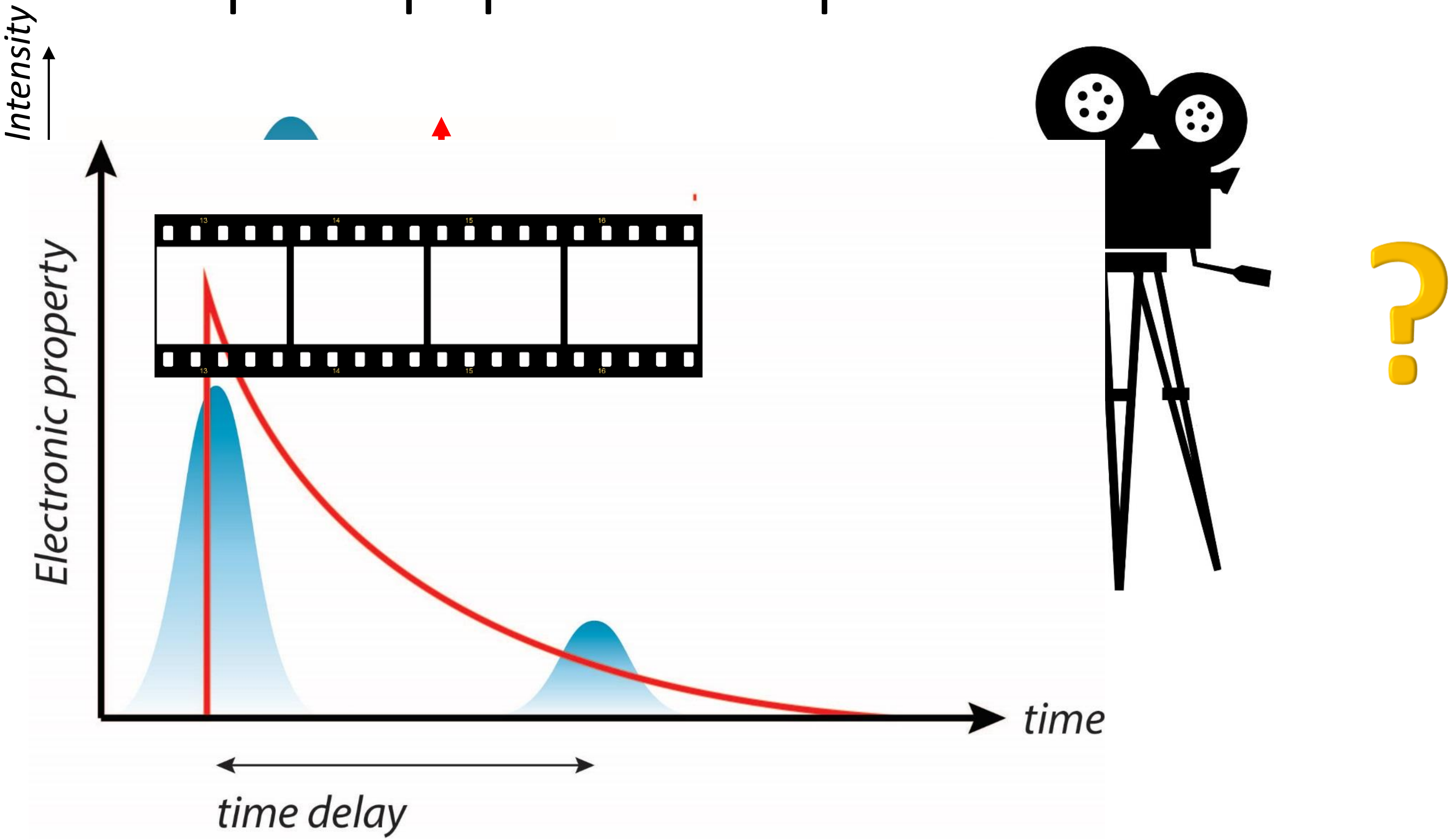
Angle-resolved photoemission spectroscopy (ARPES) [1] provides a direct view on the density of low energy electronic excited states in solids—the 2D detector of the electron analysers used in modern ARPES is just a window into momentum–energy space of 2D compounds. A snapshot through this window stores the quasiparticle spectral weight in the momentum–energy co-ordinates [2–5]. Being essentially 2D, the superconducting cuprates are a perfect example of the 'arpesable' compounds [1]. All the interactions of the electrons which are responsible for their unusual normal and energy space, even for one compound, will take ages of experimental work.

Leaving such a global task for the nearest future, one can focus on the two cuts in the Brillouin zone (BZ): nodal and antinodal directions (see Fig. 1a). These regions represent an inherent anisotropy of the electronic interactions in the cuprates which appear in anisotropy of the superconducting gap [7], pseudogap [8], and coupling strength [9] (or scattering in general). While the pronounced doping dependence of the quasiparticle spectral weight in the antinodal region of the BZ unambiguously points out to the magnetic origin of the strong electron–boson coupling seen by ARPES [9–11] (see Fig. 1c–

ARPESable: materials which easily yield good ARPES spectra

Why is Bi_2Se_3 so ARPESable?

One class of experiment with ultrafast lasers: pump-probe experiments



Pump-probe experiments

The pump

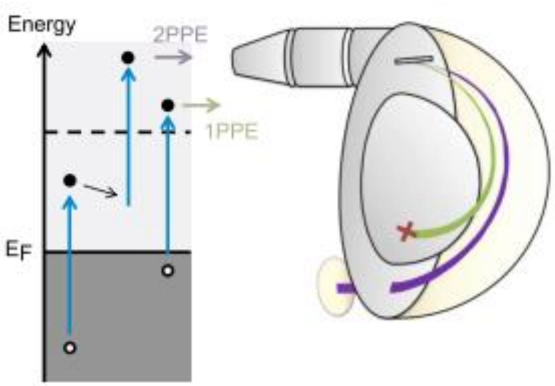
- Purpose (depends on specific experiment)
  - Create specific excitation
  - Whack the electronic system on a timescale faster than lattice response
  - Cause destruction
- Frequency (depends on specific experiment)
  - 1.5 eV (straight out of the Ti-Sapph laser)
  - Mid-IR (70-500 meV—relevant to excitations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

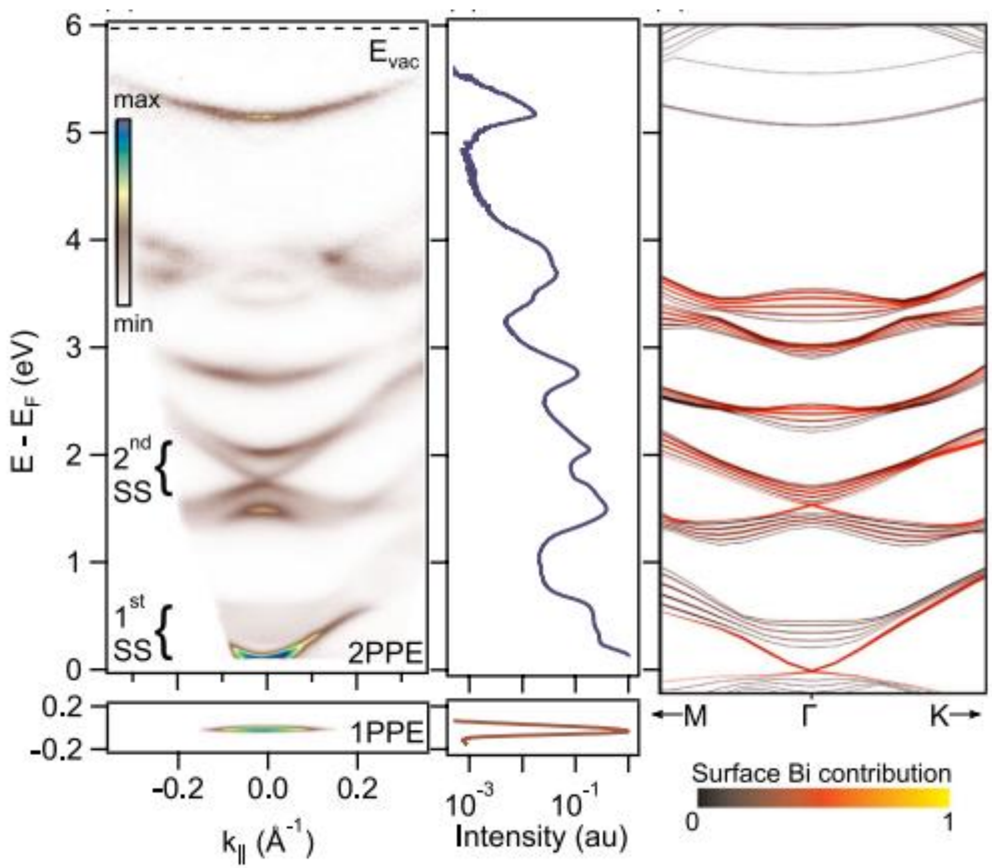
Photoemission	Photon in, electron out	Measure **occupied** electronic states	Sub-meV resolution common
Inverse photoemission	Electron in, photon out	Measure **unoccupied** electronic states	~500 meV resolution



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^{nd} order process

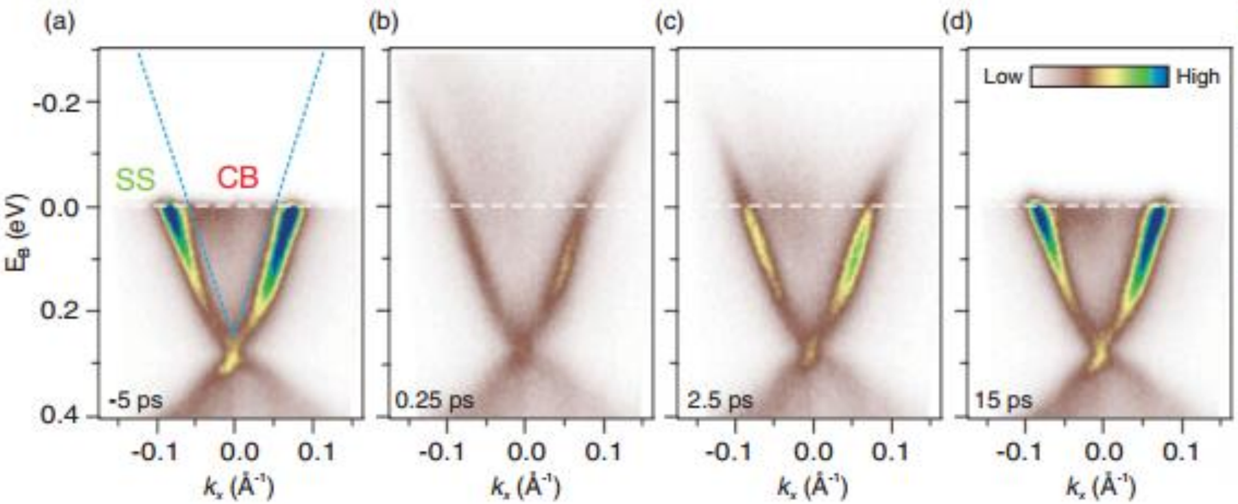
2 PPE experiments in Bi_2Se_3

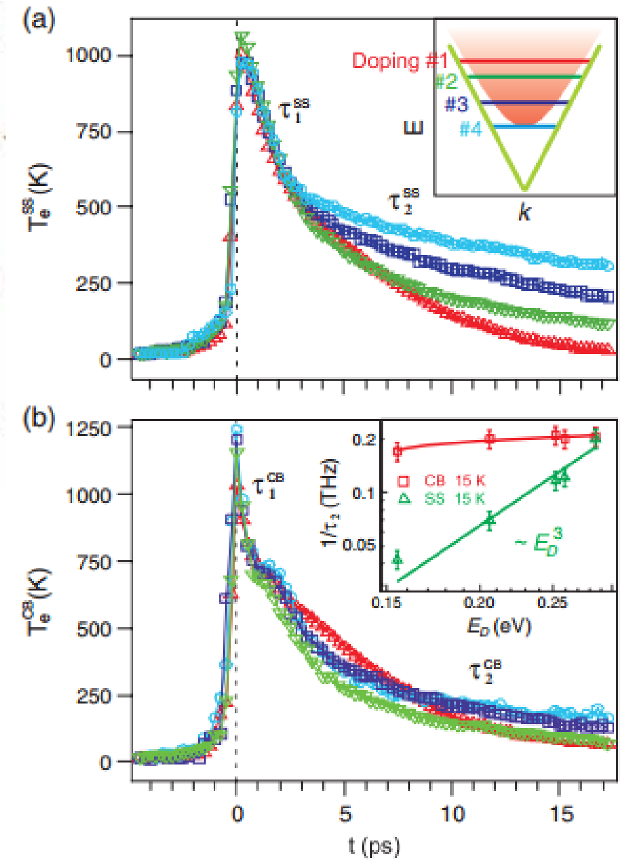


- 1.5 eV pump, 5.98 eV probe, $\Delta t \sim 100 fs$
- 2nd surface state observed above E_F!
- Applicable to many different materials

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

$$H(t+T) = H(t)$$

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

$$\phi_\alpha(t) = \phi_\alpha(t+T)$$

$$\epsilon_\alpha \text{ and } \epsilon_\alpha + n\hbar\omega$$

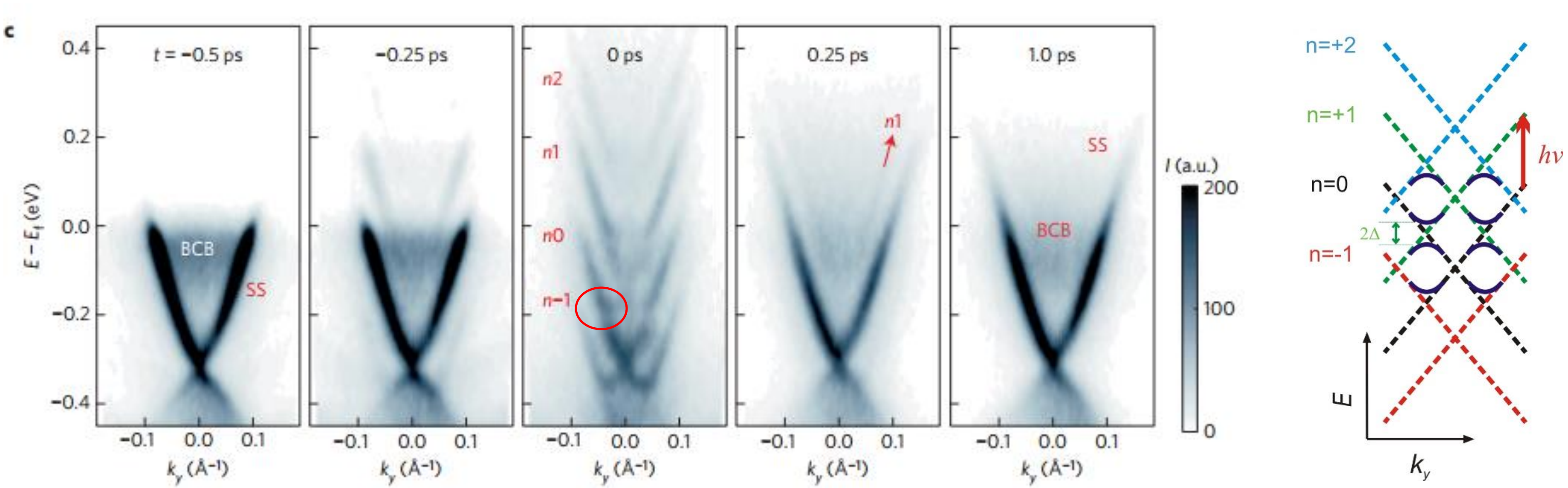
$$(\omega = 2\pi/T)$$

If you have both spatially and temporally periodic Hamiltonian, Eigenvalues are periodic both in k and E! -> Floquet-Bloch states!

Slide courtesy of N. Gedik

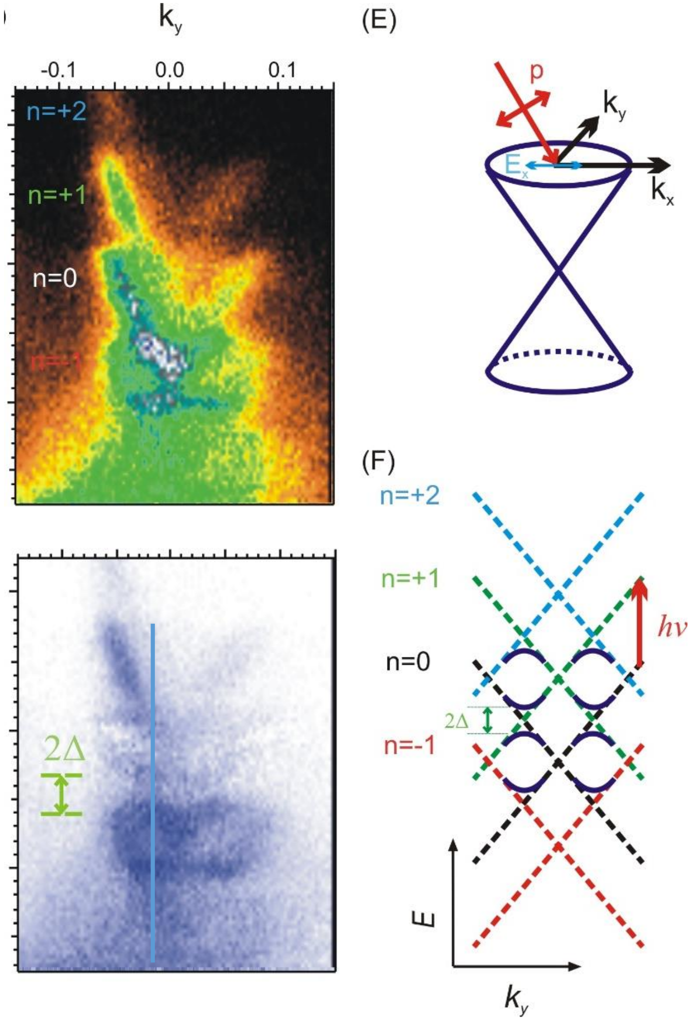
Creating new states of matter with light

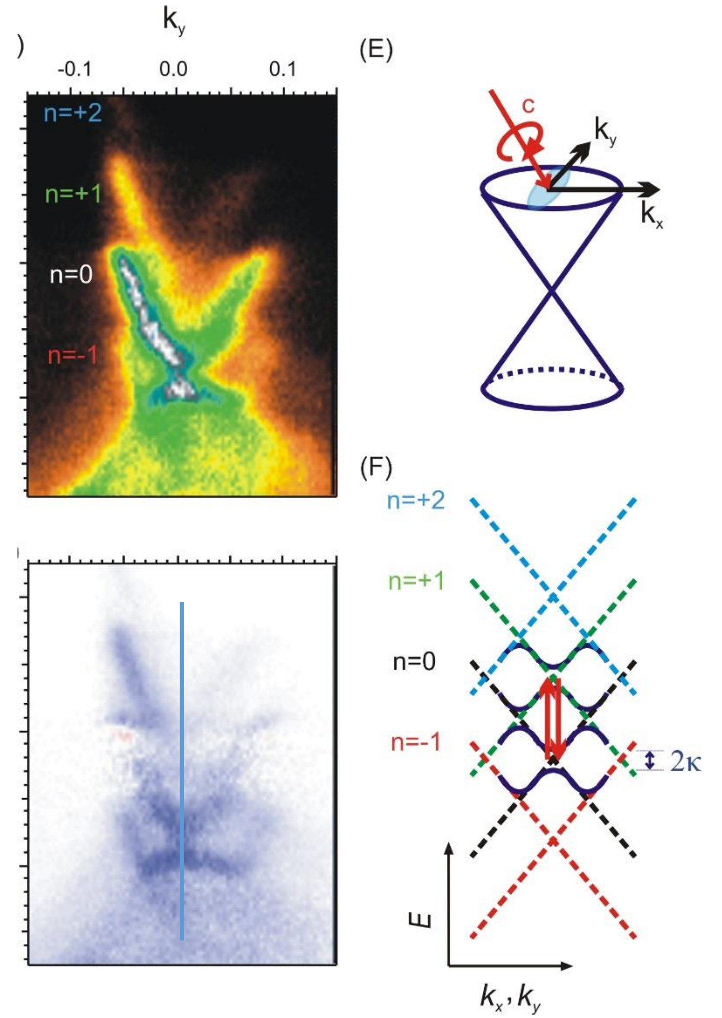
- Use mid-IR pump with energy **smaller** than band gap of Bi2Se3
- Use oscillating electric field of pump to create floquet-bloch state
- Photoinduced gaps at band crossings
- Circularly polarized light can open gap at Dirac point!



Wang *et al.* Science **342** 514 (2013)
Mahmood *et al.* Nat. Phys. **12** 453 (2016)

Opening gaps with light!





Wang *et al.* Science **342** 514 (2013)

Conclusions part 2

- Bi_2Se_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

- H. Zhang *et al.* Nat. Phys. **5** 438 (2009)
- J. E. Moore *et al.* Nature **464** (2010)
- Qi and Zhang *Phys. Today, "The quantum spin hall effect and topological insulators"* Jan (2010)