Surface States of Rashba Spin-Split Type and Topological Insulators

Bi： Bulk = Semi-metal,
Surface =Spin-split metal (Rashba effect)

$Bi_{1-x}Sb_x$, Bi_2Se_3 ↓
: Bulk = Insulator (Topological Insulator)
Surface = Spin-split metal (Topological Metal)

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[4] HSRC [5] Julich, Germany [6] San Sebastian, Spain

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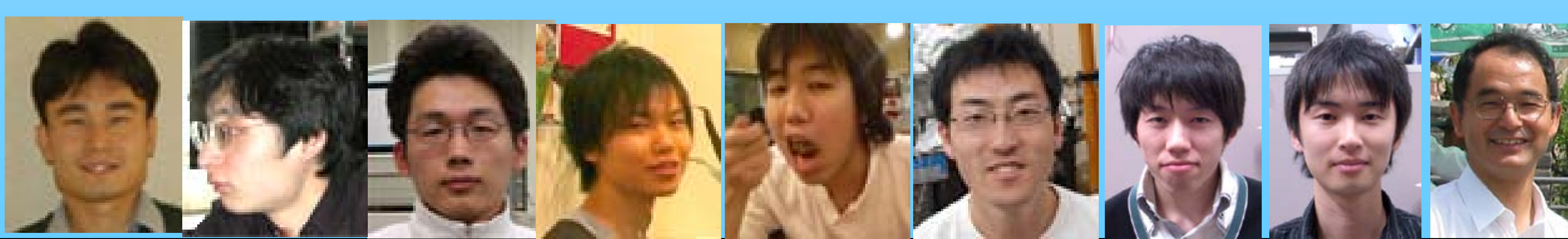
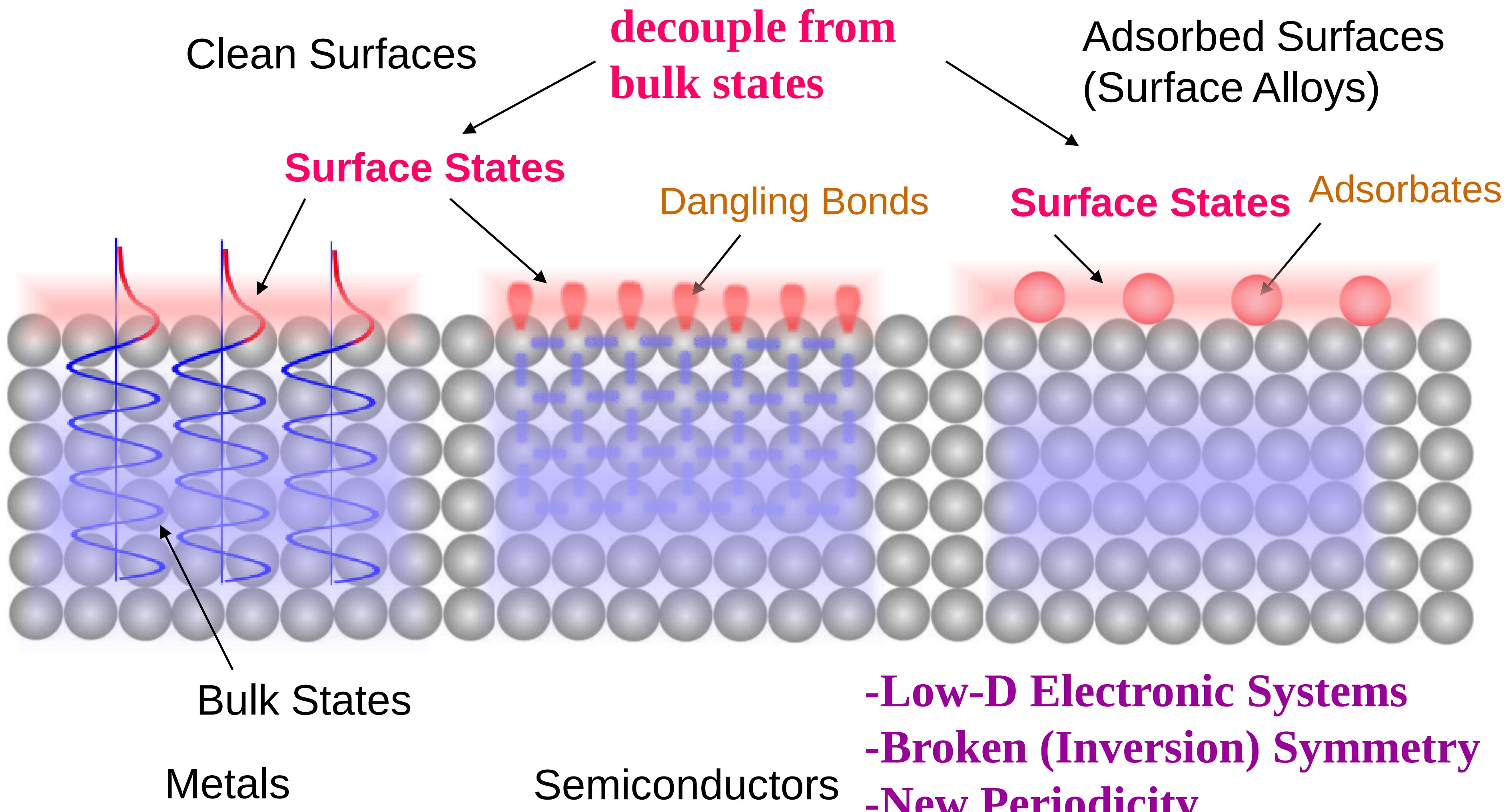
S. Kimura,[2] T. Okuda,[3,4] G. Bihlmayer,[5] E. V. Chulkov[6] , S. Hasegawa[1]

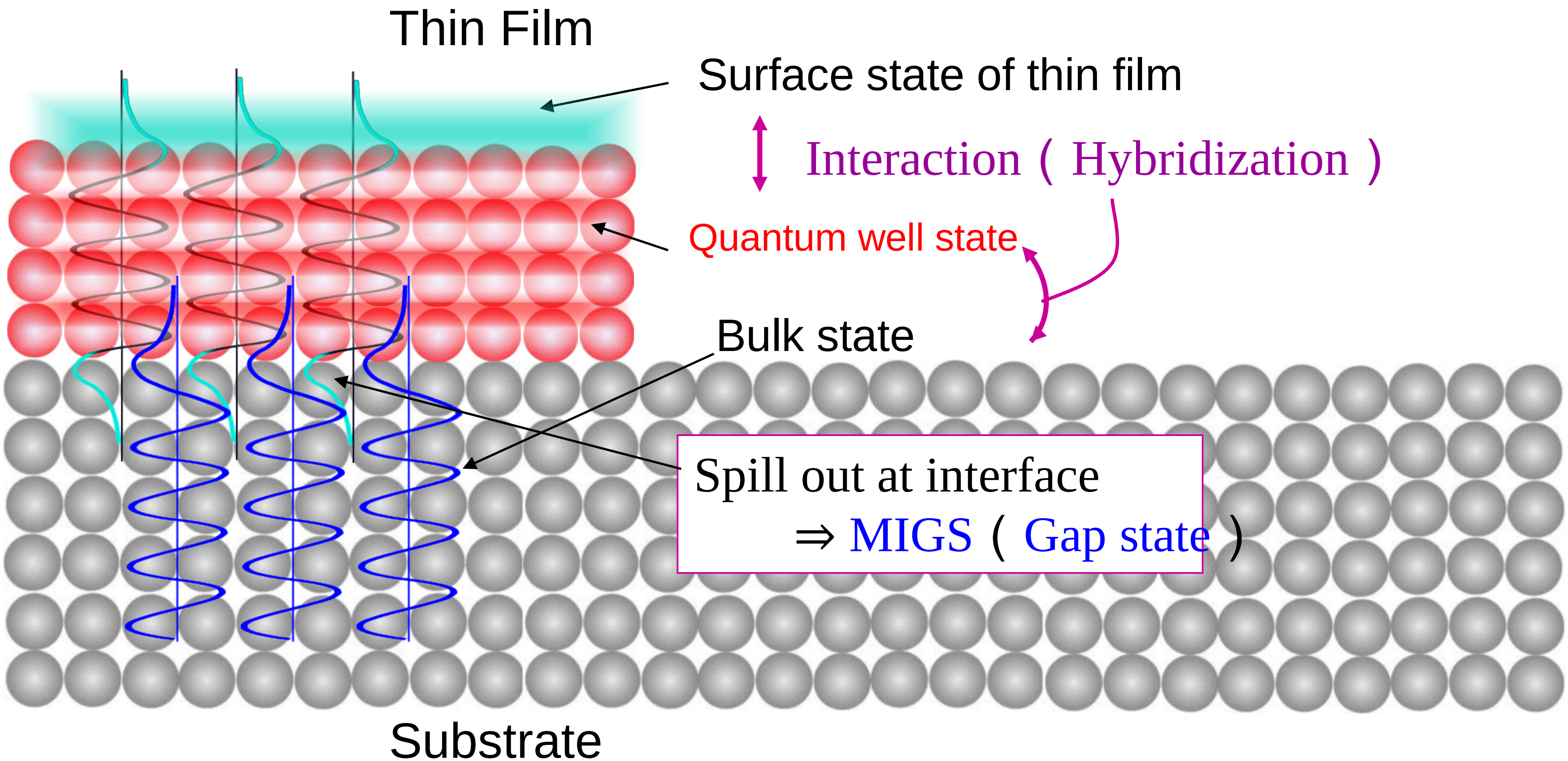


Surface States — Shockley & Tamm States —



- -Low-D Electronic Systems
- -Broken (Inversion) Symmetry
- -New Periodicity

Thin Film and Interface



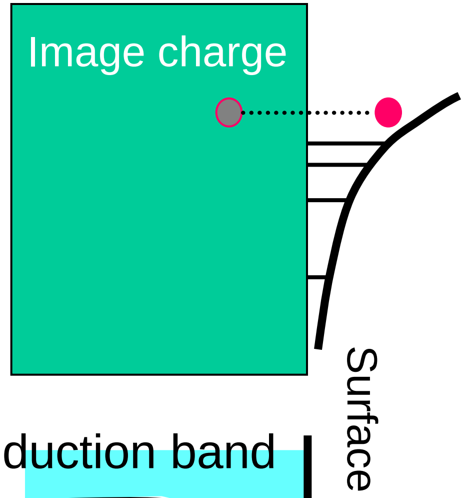
Ex: Interaction between QWS and surface state

QWS's are spin-split

← Spin-split surface state due to Rashba-effect

K. He, et al., PRL **101**, 107604 (2008)

Various Surface States



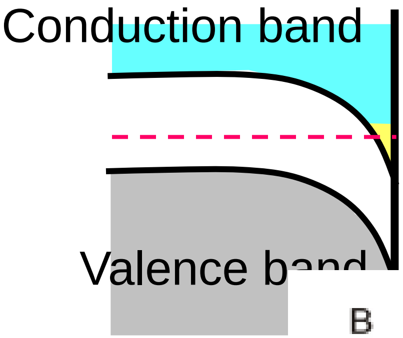
1. Shockley states (extended)
   Tamm states (localized)

   Chemical bonding, Potential

   (Previous slide)

2. Image states

   Image charge



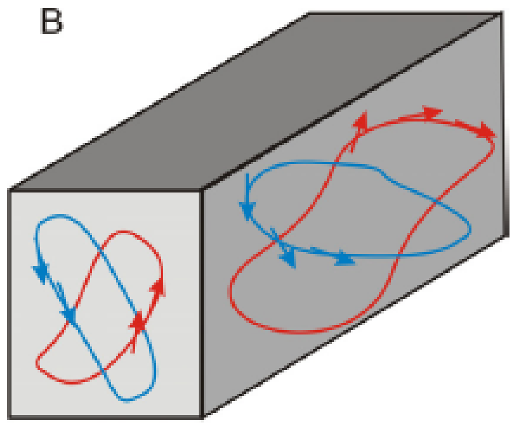
3. Surface space-charge layer

   Bending of bulk bands

4. Topological surface states

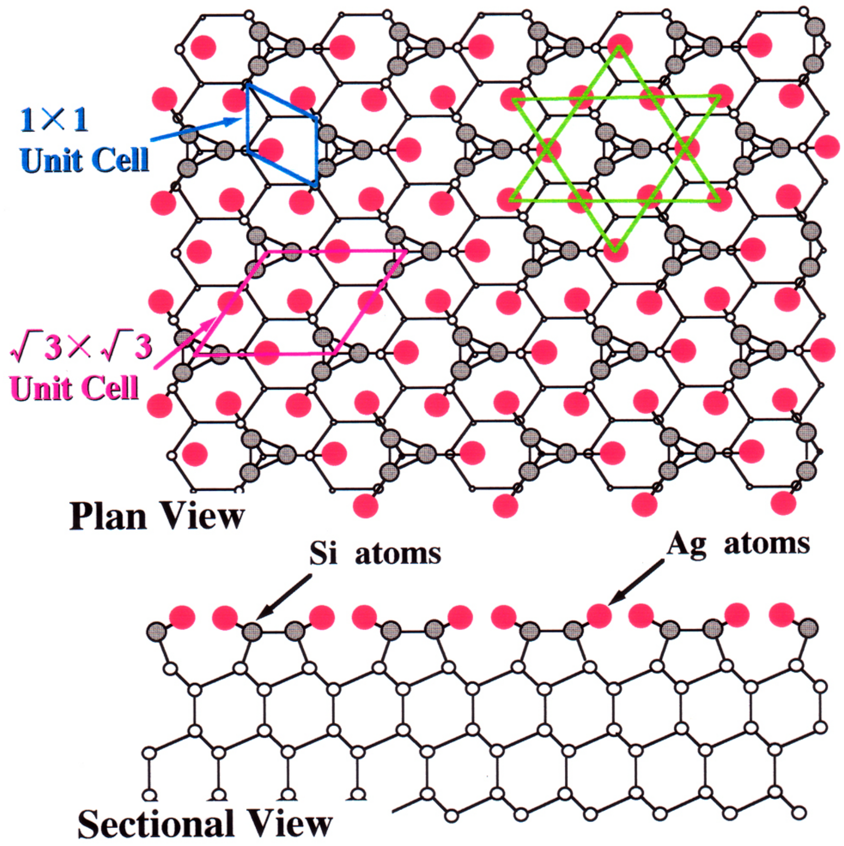
   Spin-orbit coupling ← Edge states of Q(S)H phase

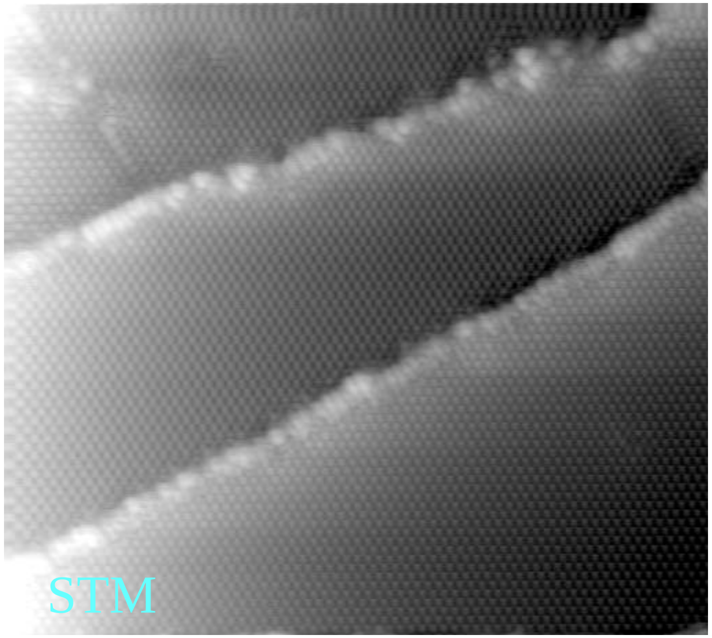
   HgTe (QW), $Bi_{1-x}Sb_x$, Bi_2Te_3, Bi_2Se_3,



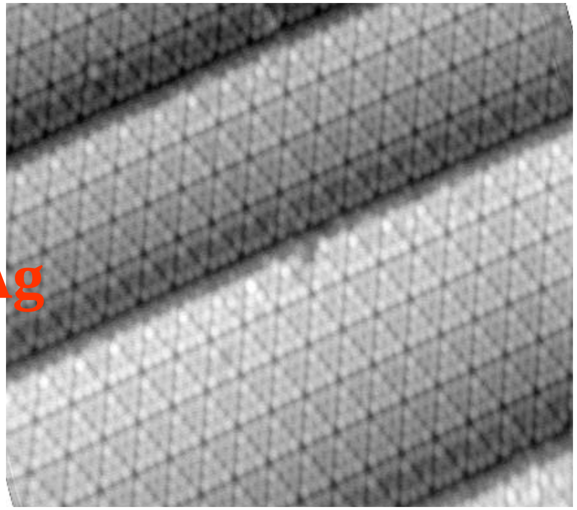
MonAtomic Layer of Ag: Si (111)-√3×√3-Ag Surface

2D Metal





Deposit Monolayer of Ag



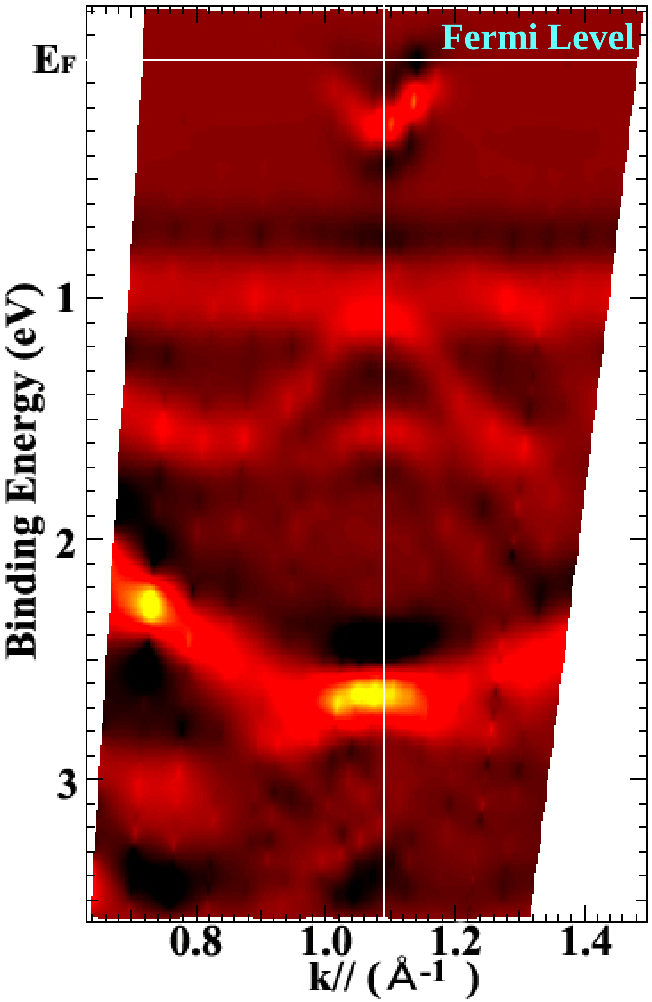
Clean Si(111)-7x7

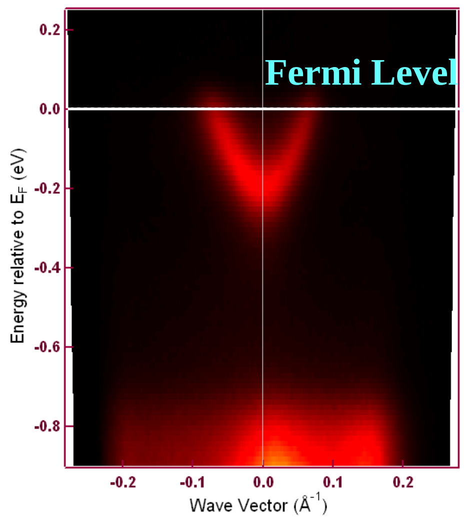
Surface-state bands of Monolayer Ag : Si(111)-√3x√3-Ag

ARPES

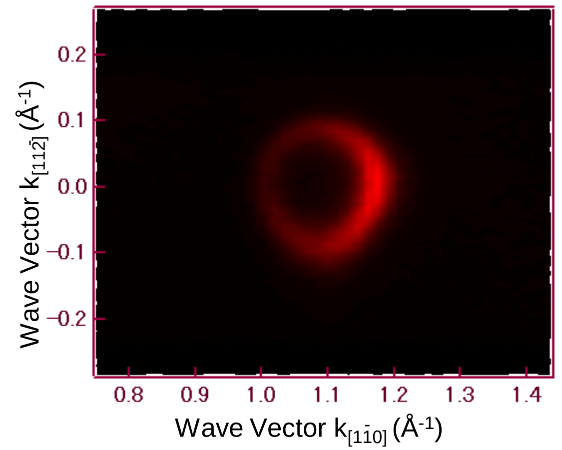
S. Hasegawa, *et al*., Prog. Surf. Sci. **60** (1999) 89.
T. Hirahara, *et al*., e-J. Surf. Sci. Nanotech. **2** (2004) 141.
T. Hirahara, *et al*., Surf. Sci. **563** (2004) 191.

Band Dispersion

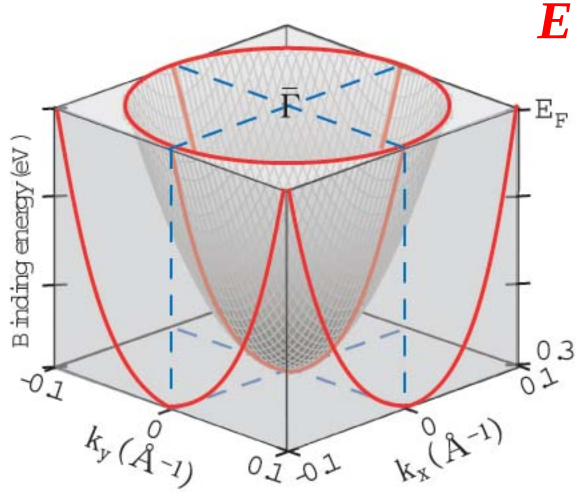




Fermi Surface Mapping



$m^*=0.13m_e$



Parabolic Dispersion

$$E = \frac{\hbar^2 k^2}{2m^*} \longrightarrow$$

Free-electron

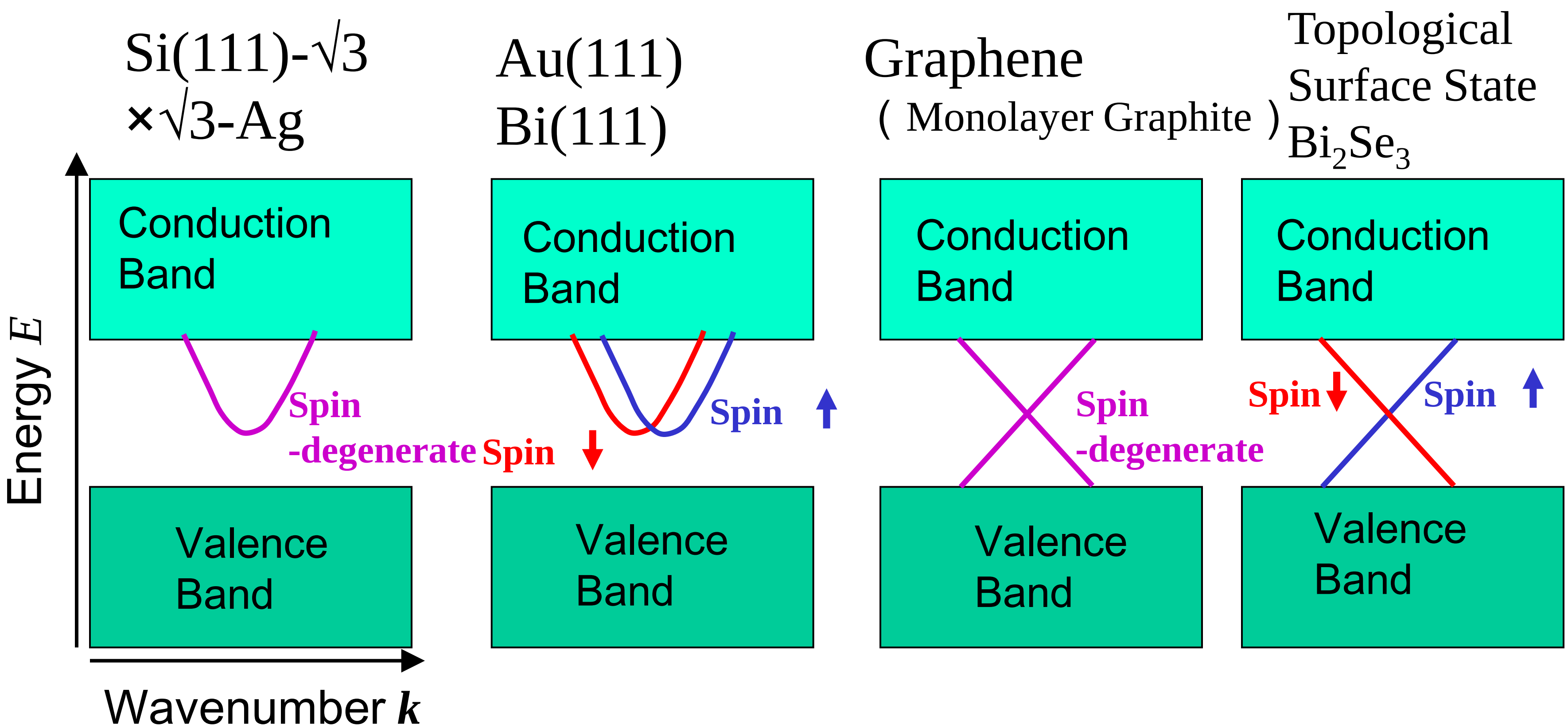
Metallic

Fermi Circle

↓

Isotropic, Metallic,
Free-electron-like
Surface state

Various Surface Sates



$$E = \frac{p^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*}$$

Free-Electron-like

$$E = \sqrt{(mc^2)^2 + (pc)^2}$$

$$m = 0$$

$$E = \pm pc = \pm c\hbar k$$

Massless Dirac Fermion

Rashba Effect in Surface States

E. I. Rashba,
Sov. Phys. Solid State **2**, 1109(1960)

$$H = \frac{1}{2m}p^2 + V(x) + \frac{1}{4mc^2}\sigma \cdot \left(gradV(x) \times p \right)$$

Spin-orbit coupling Hamiltonian

Symmetry

Time reversal symmetry
E(*k*, ↑)=E(- *k*, ↓)

~~**Inversion symmetry**~~
~~**E(*k*, ↑)=E(- *k*,↑)**~~

Bloch theory
E(*k*+*G*, ↑)=E(*k*,↑)

Kramers Degeneracy

E(*k*, ↑)≠E(*k*, ↓)

E(G/2, ↑)=E(G/2, ↓)

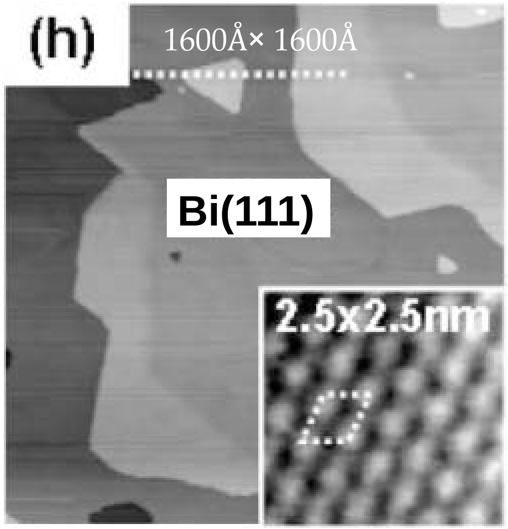
Only at some symmetric points

Atomically Flat Ultrathin Bi Film on Si(111)-7×7

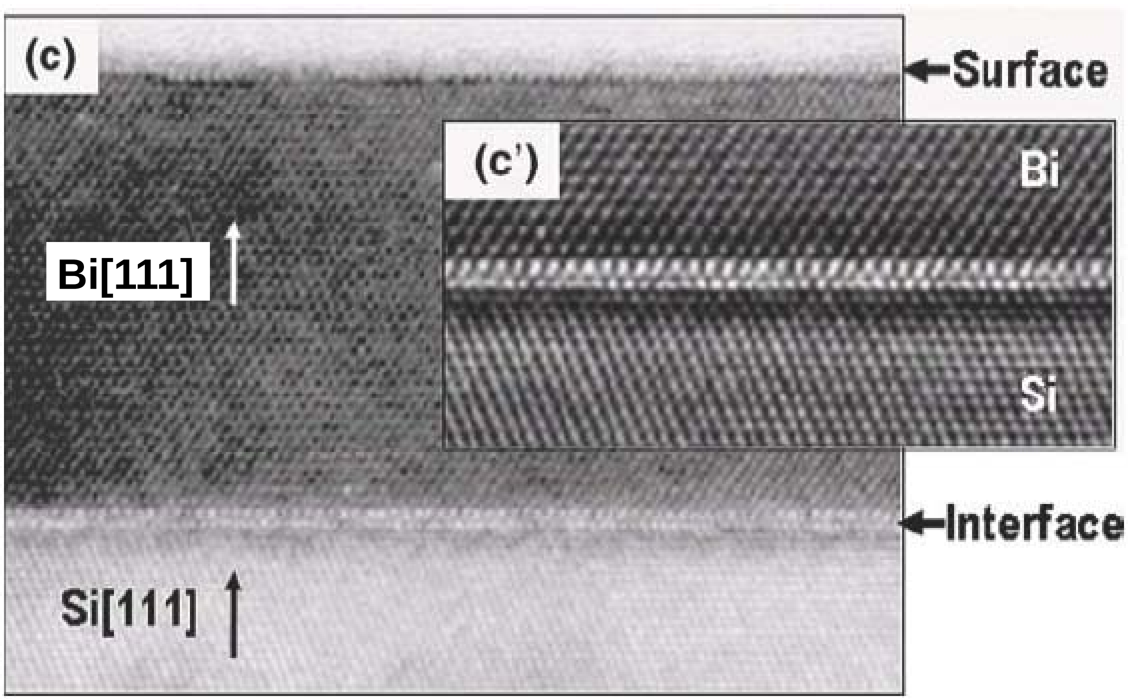
T. Nagao *et al.*, PRL **93** 105501(2004)

T. Nagao *et al.*,
Surf. Sci. **590**, L247-252 (2005).

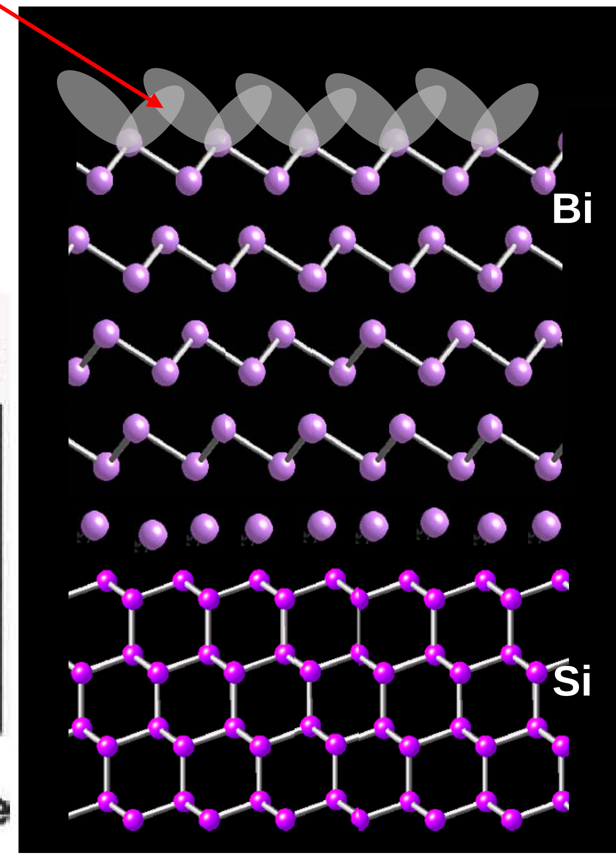
STM



XTEM



Surface States



ARPES：
Electronic States of Bi Quantu

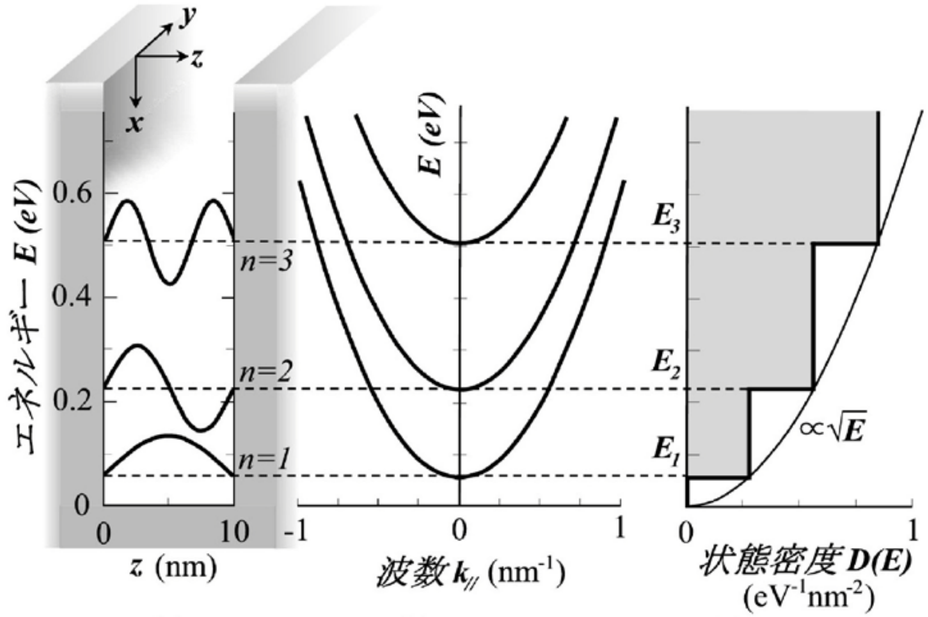
T. Hirahara, et al., PRB **75**, 035422 (‘07)

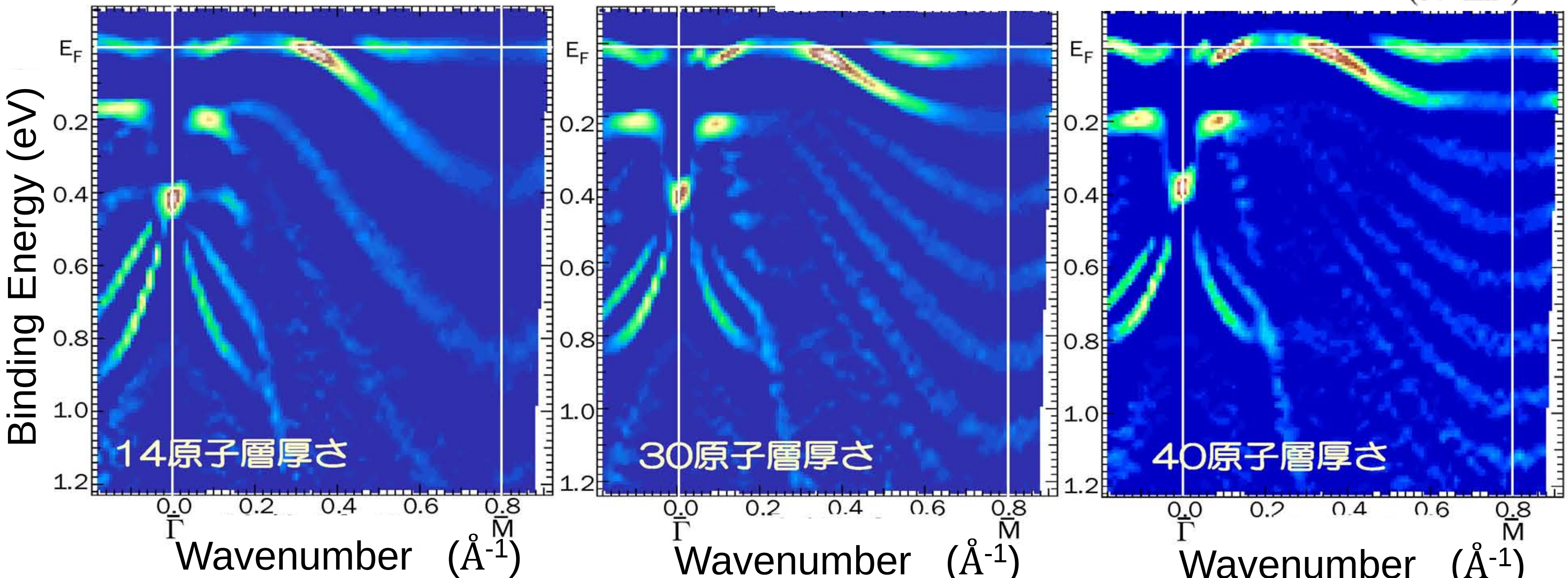
Quantum-Well States

Surface States ：

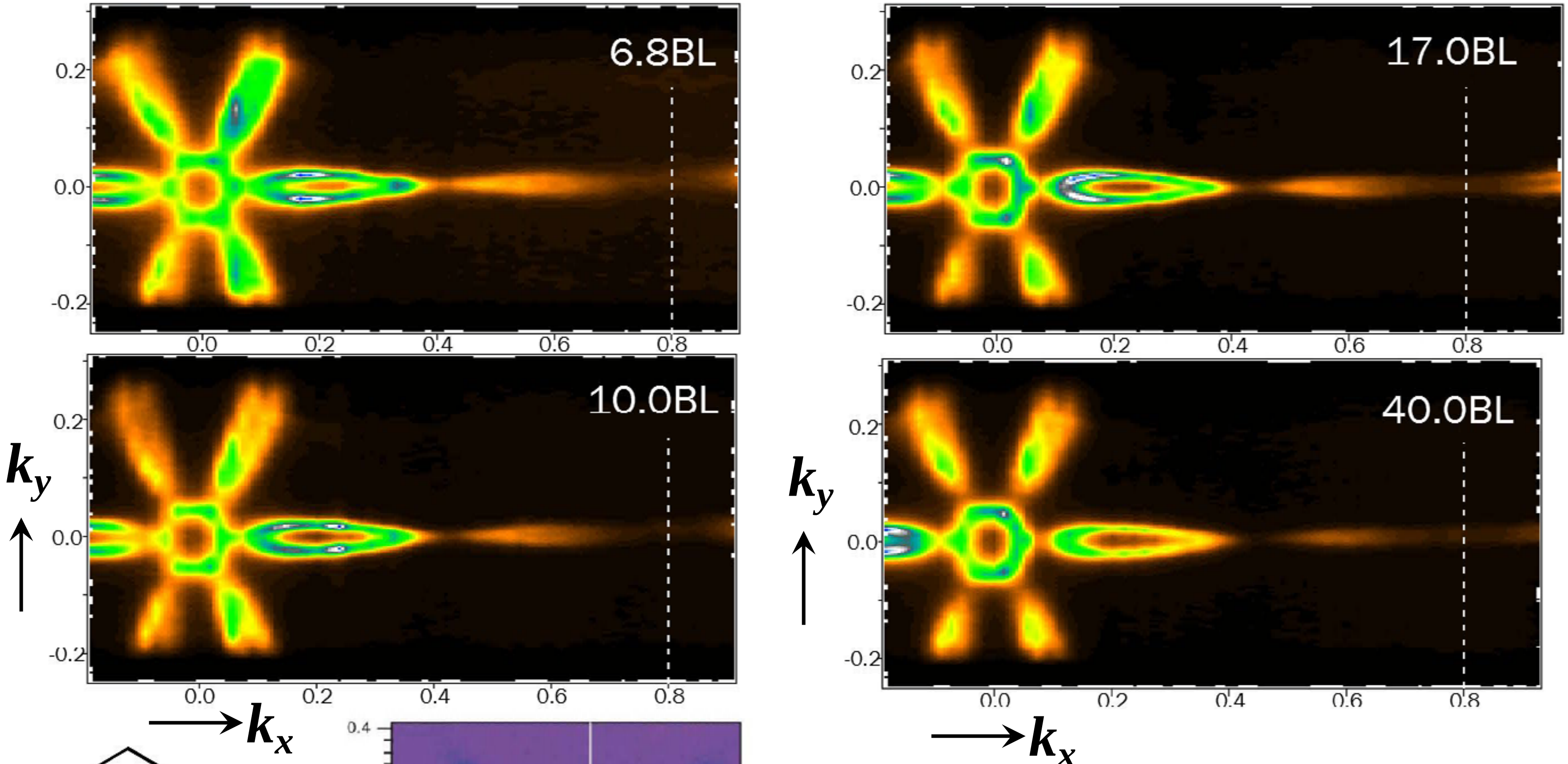
Electrical Cond. Of Bi Film

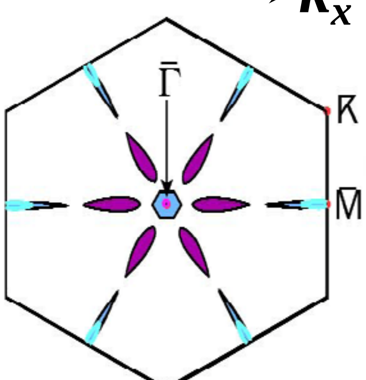
= Surface-State Conduction

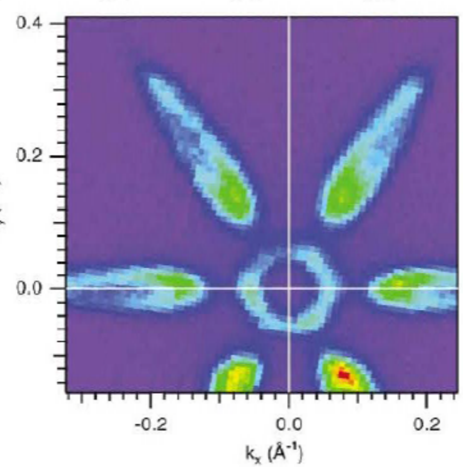




Fermi Surfaces of Bi(001) films







No thickness dependence

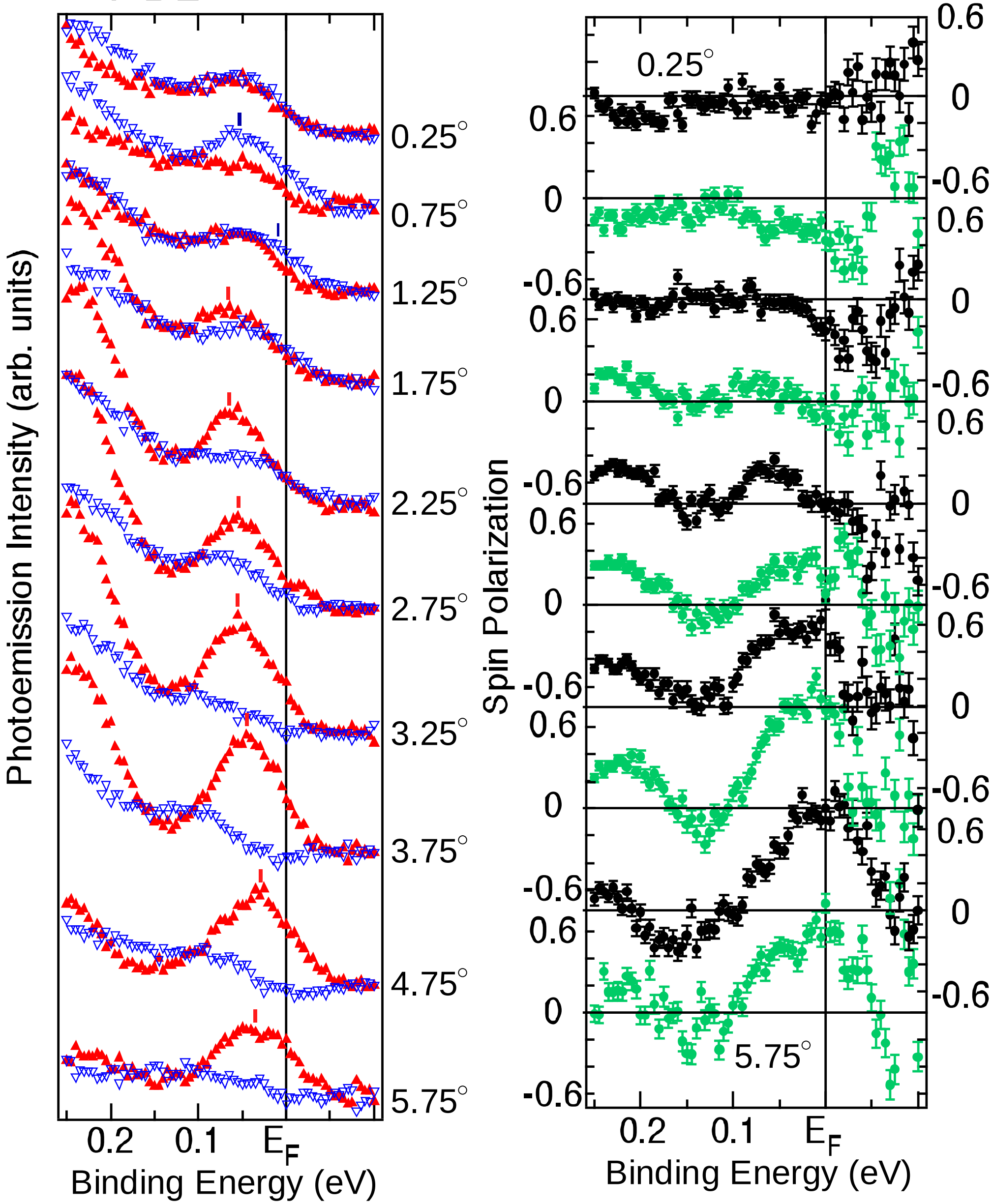
Highly metallic

Same as those of single crystal Bi

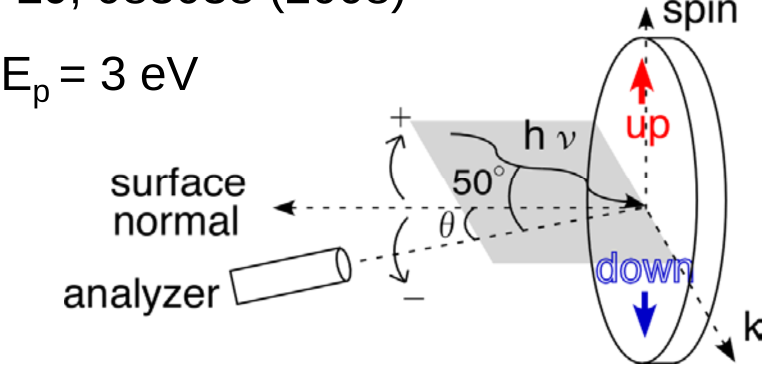
Single Crystal of Bi: C. R. Ast *et al.*, PRL **87** 177602(2001)

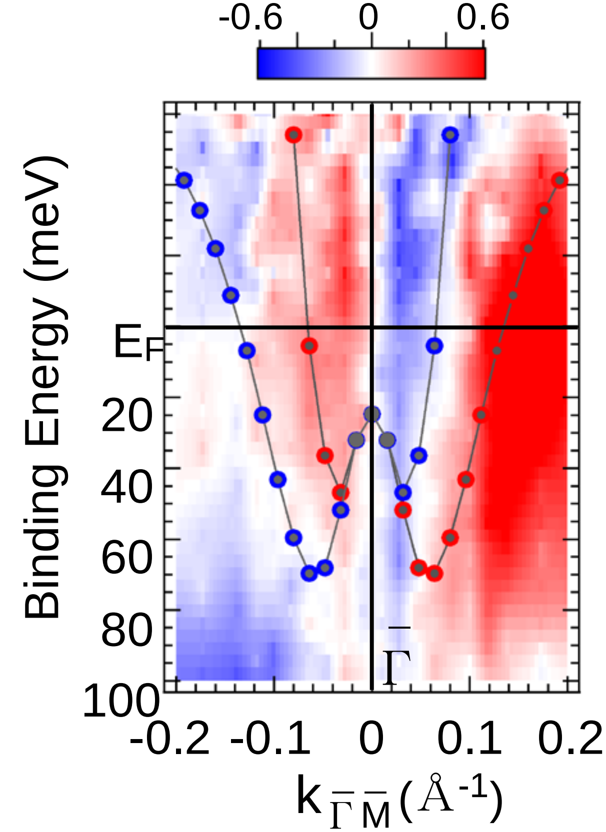
Spin-resolved ARPES

T. Hirahara, et al., New J. Phys. **10**, 083038 (2008)



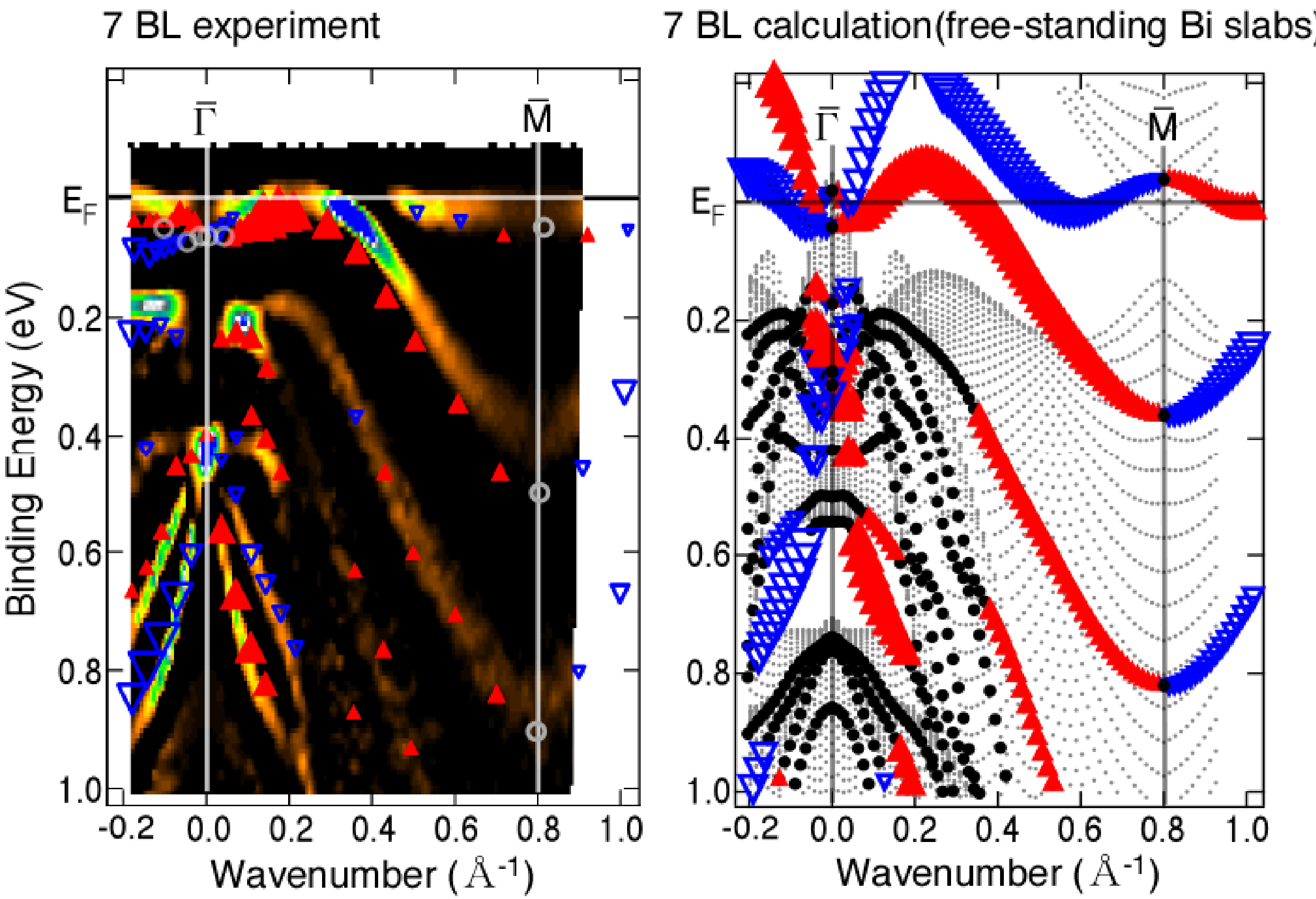
max ~ +0.75





Consistent with the Rashba model

Spin-resolved band mapping



Size of the markers

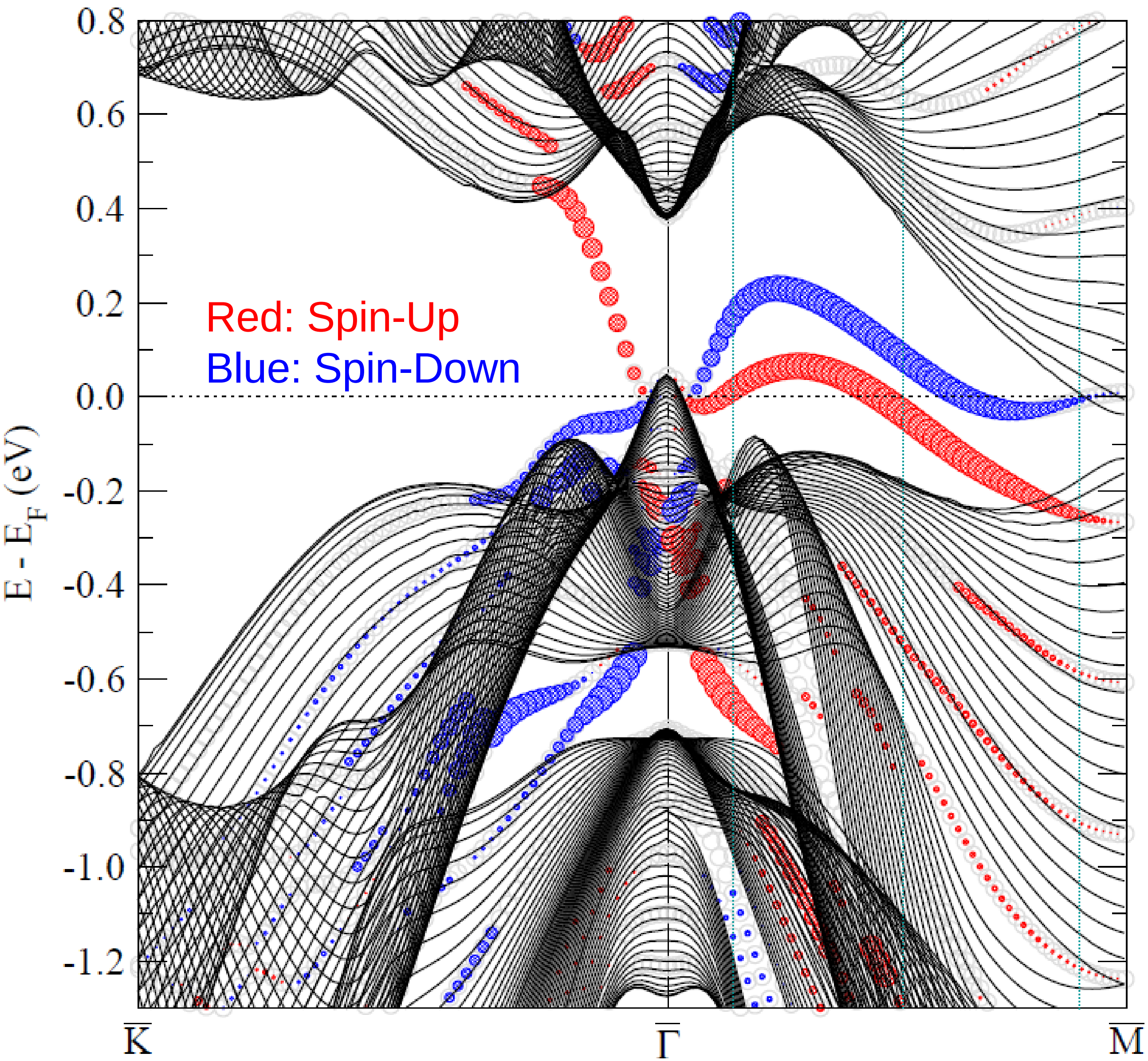
||

Magnitude of the spin polarization

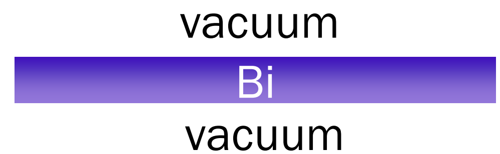
Asymmetric spin structure with respect to $\bar{\Gamma}$ and $\bar{M}$

Qualitative consistency between experiment and calculation concerning the k-dependence of the spin polarization

Dispersion of a symmetric 10BL Bi slab



Bihlmayer
(Juhlich, Germany)



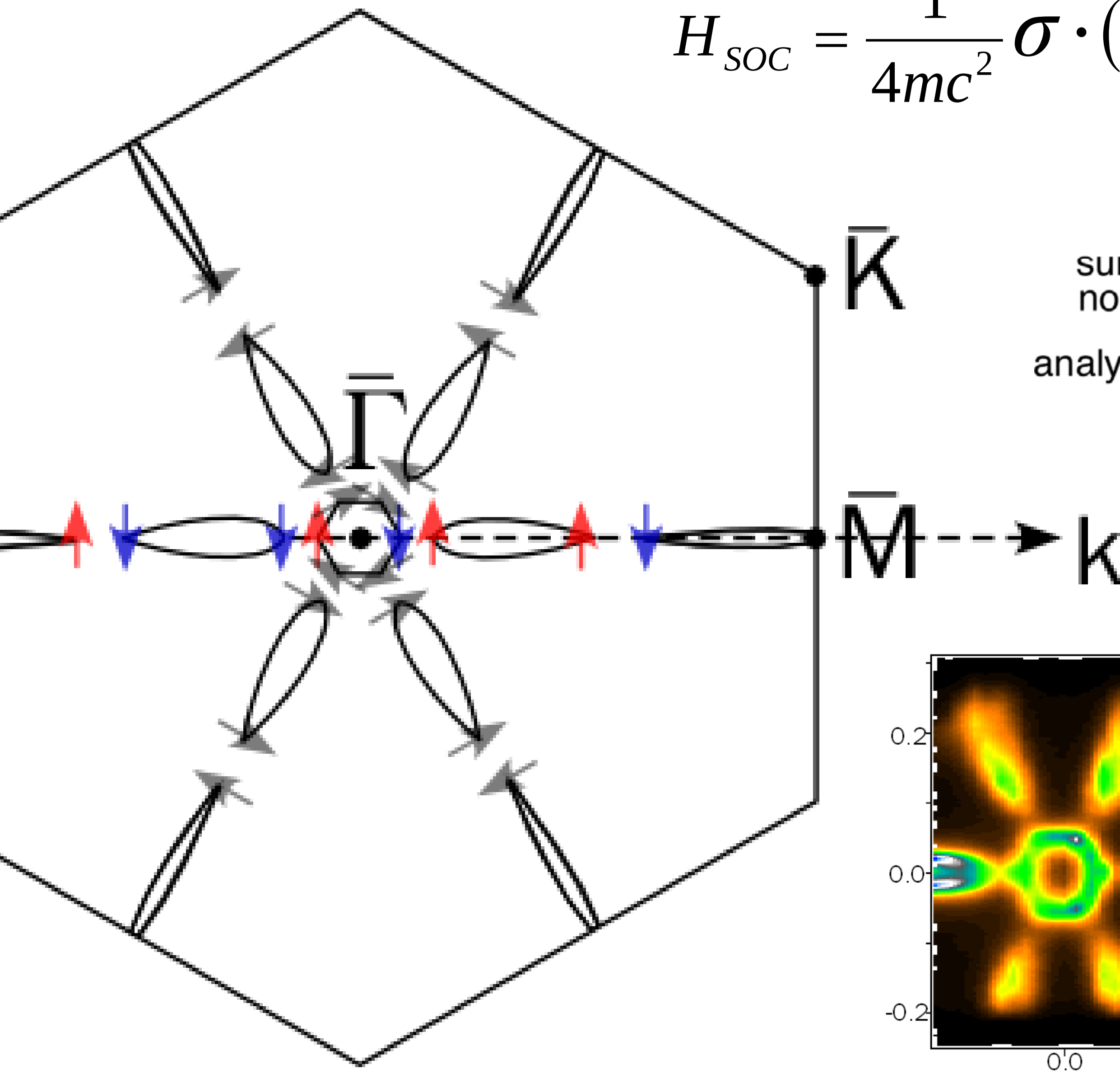
First-principles calculation for free-standing Bi slabs including SOC

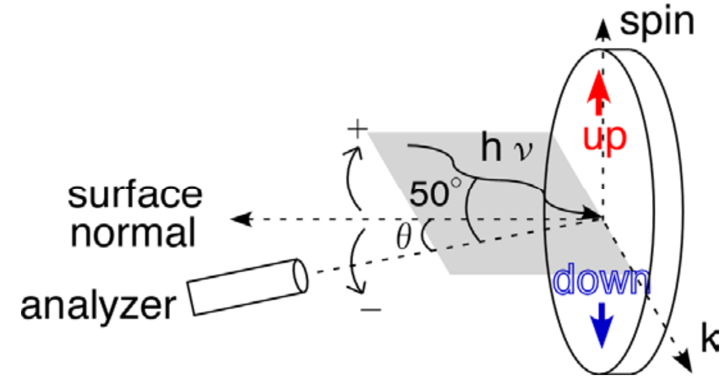
Pure Bi

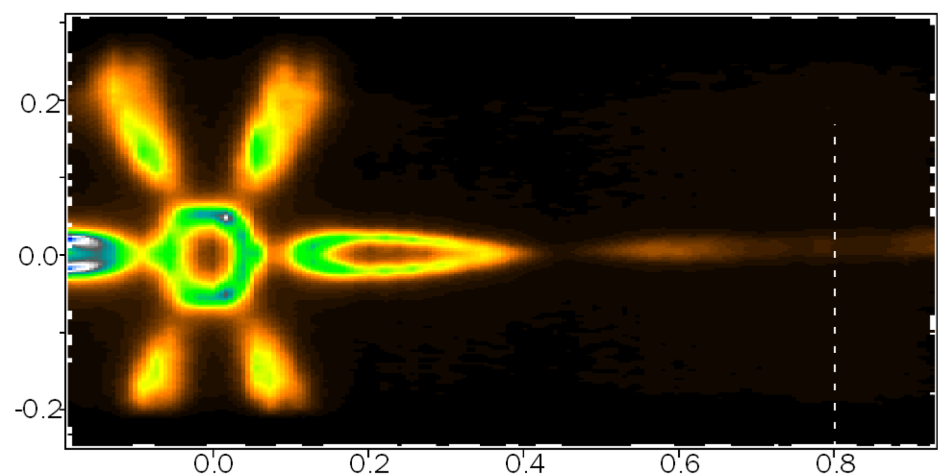
- Semi-metal in Bulk
- Conduction band and valence band are connected by the spin-split surface states

Spin-Texture Structure in Fermi Surface

$$H_{SOC} = \frac{1}{4mc^2}\boldsymbol{\sigma}\cdot\left(gradV(x)\times p\right)$$

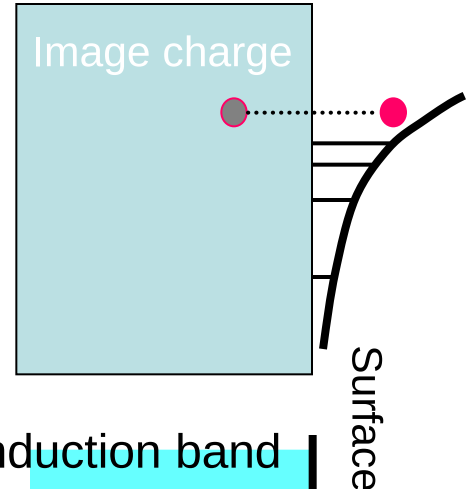




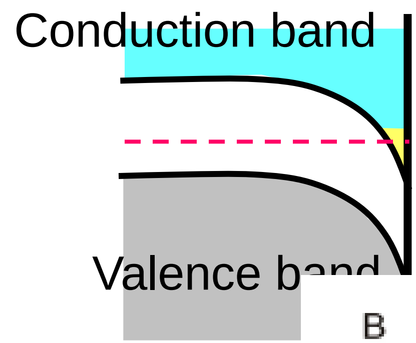


Various Surface States

1. Shockley states (extended)
   Tamm states (localized)
   Chemical bonding, Potential
   (Previous slide)

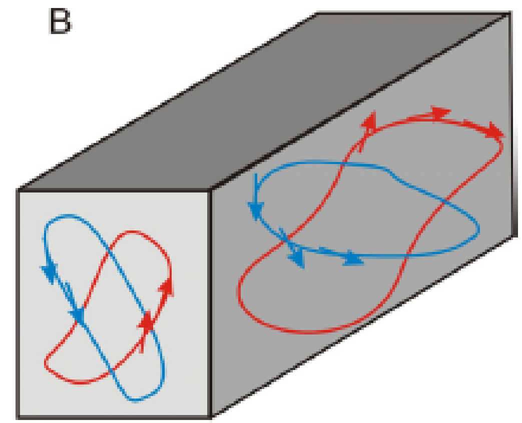


2. Image states
   Image charge



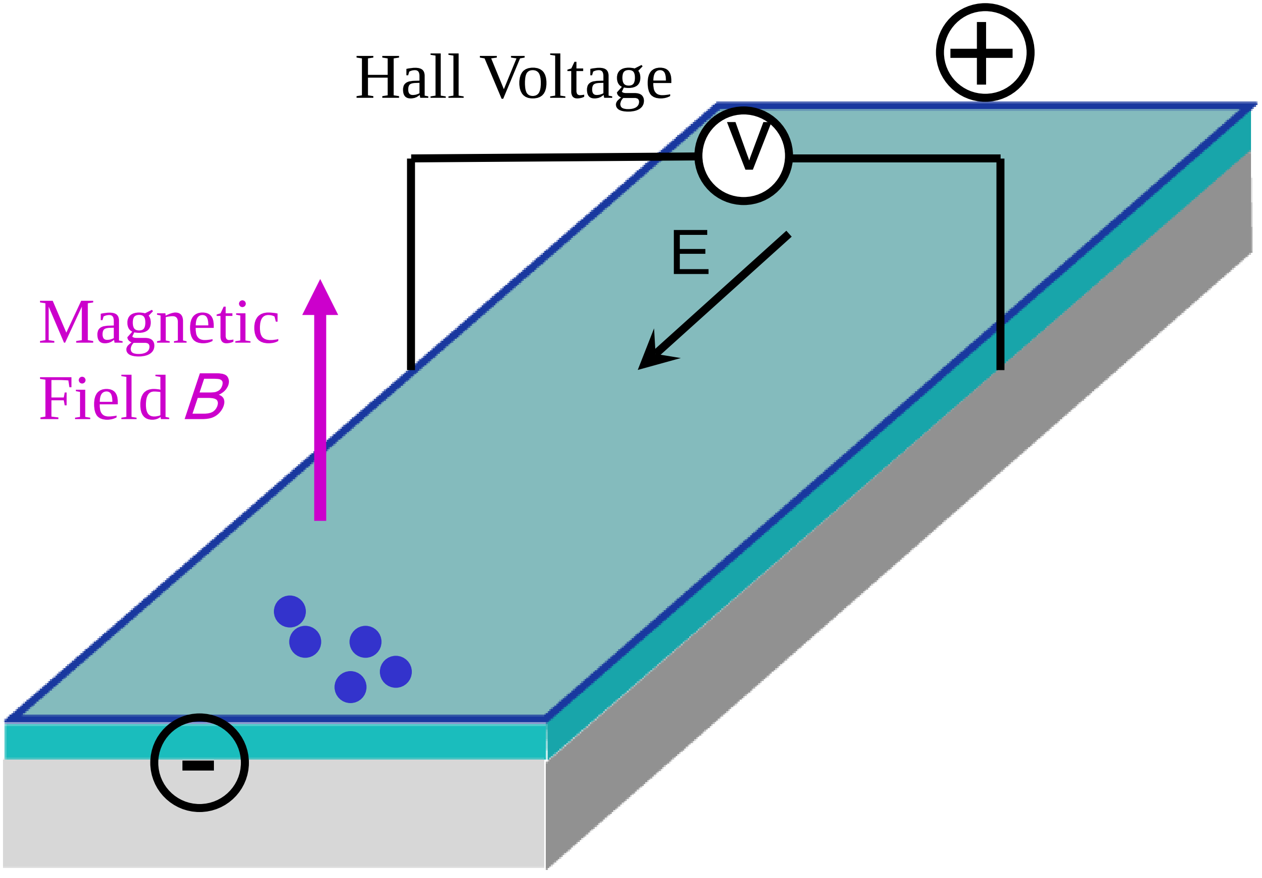
3. Surface space-charge layer
   Bending of bulk bands

4. Topological surface states
   Spin-orbit coupling ← Edge states of Q(S)H phase
   HgTe (QW), $Bi_{1-x}Sb_x$, Bi_2Te_3, Bi_2Se_3,



Hall Effect

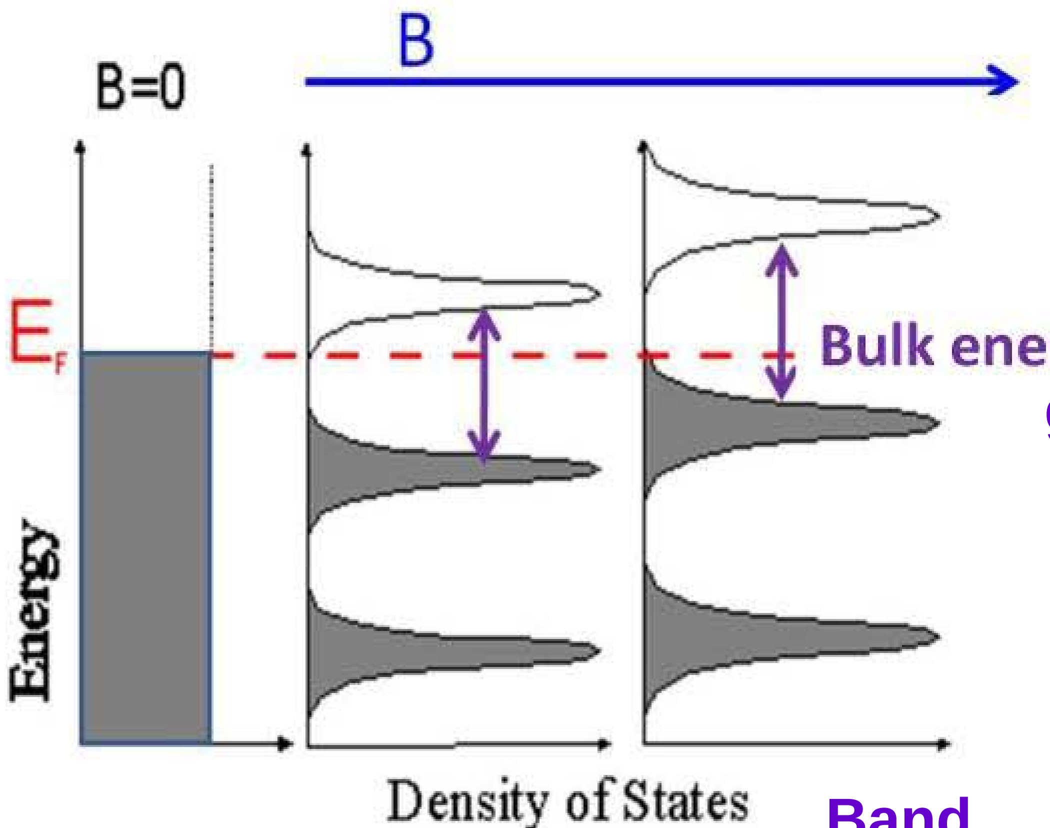
Edwin H. Hall (1879)



Hall Effect at **high** magnetic fields

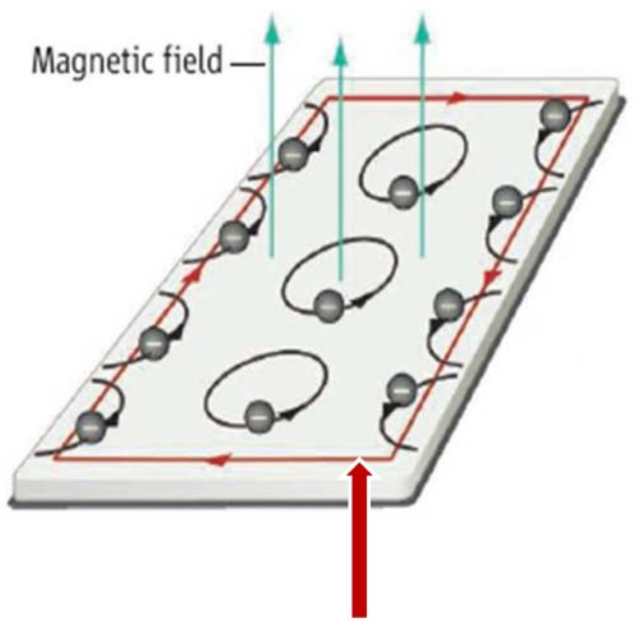
Electrons + strong magnetic field → Discrete Energy Levels

Landau Levels



Bulk energy gap

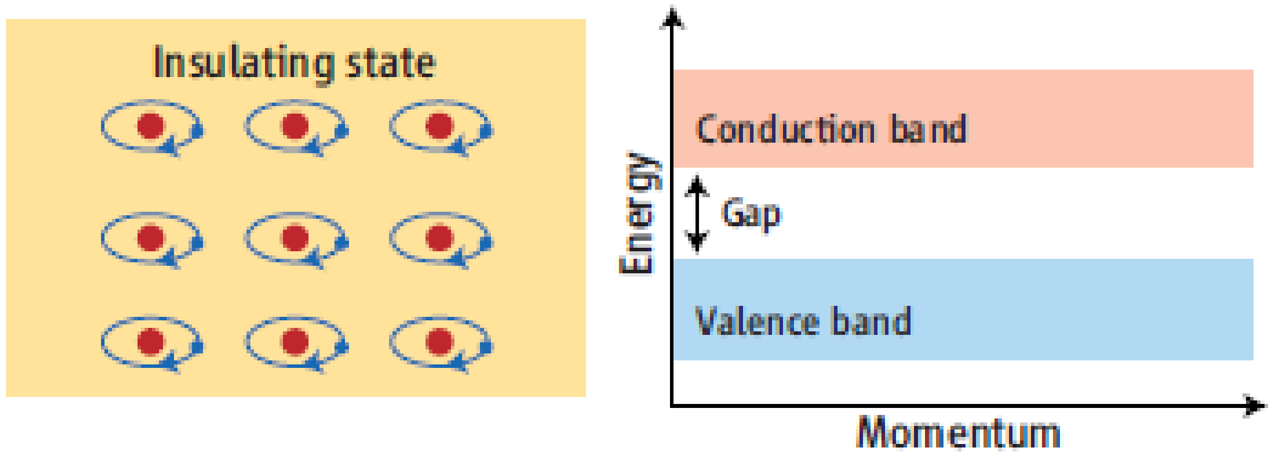
Band Insulator



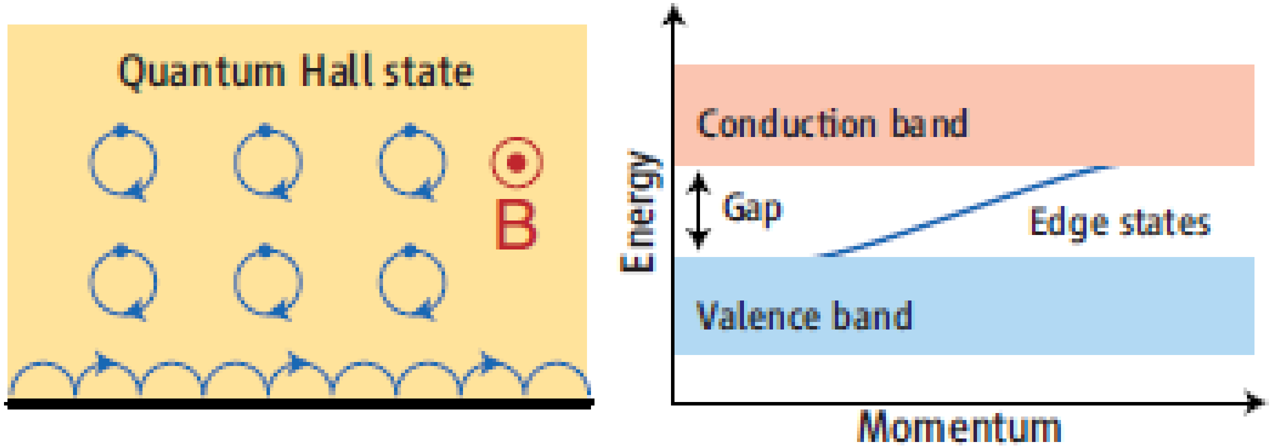
Conduction through the boundary

→Metallic edge state

Usual Band Insulator



Quantum Hall Sate



Spin Hall Effect

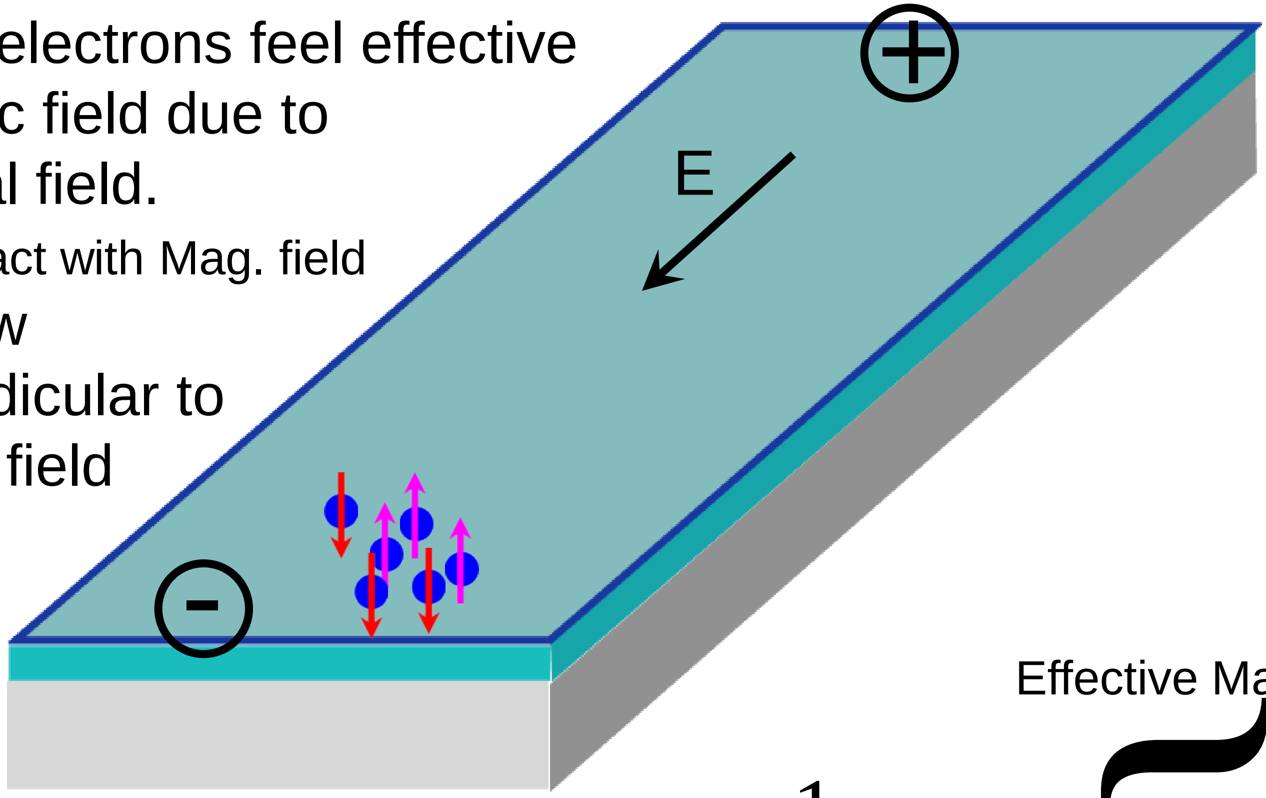
Without external magnetic field
Non-magnetic materials

Spin-Orbit Interaction

⇒Moving electrons feel effective magnetic field due to electrical field.

⇒Spin interact with Mag. field

⇒Spin flow perpendicular to electric field

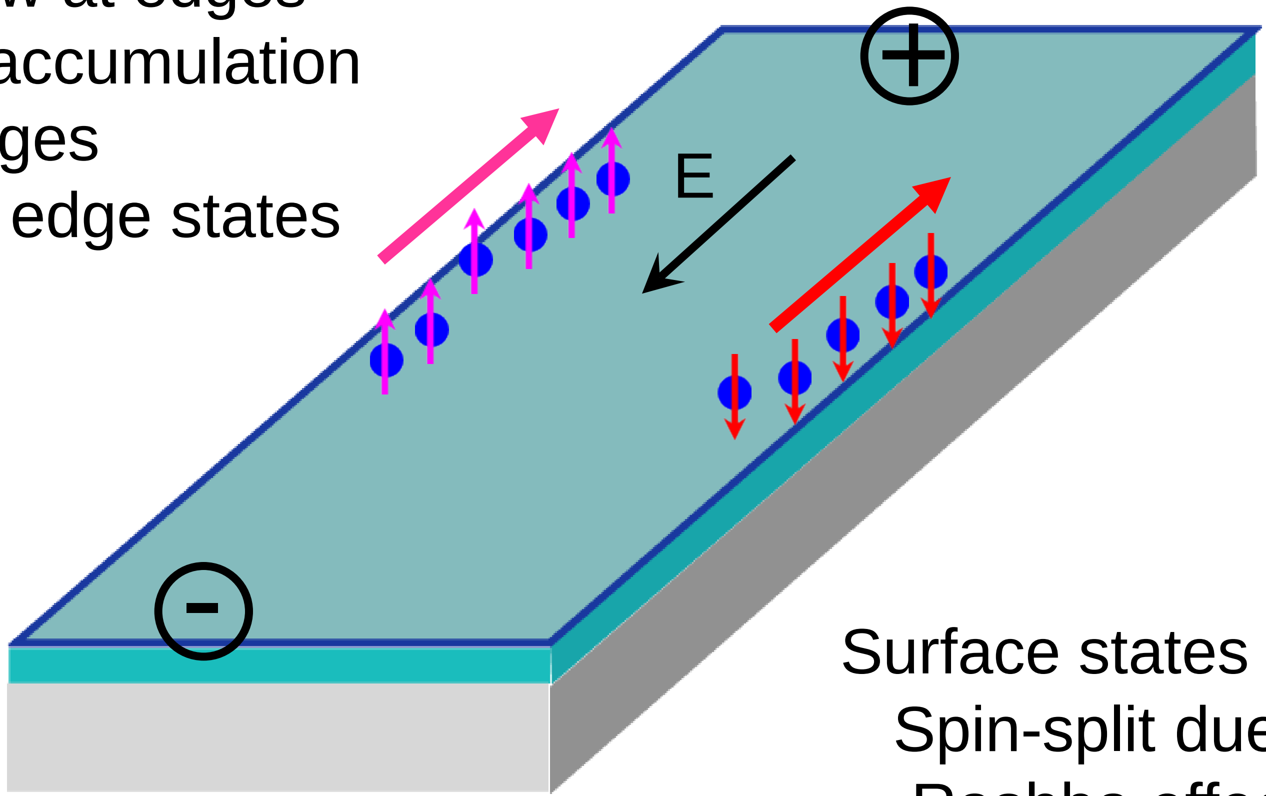


Effective Magnetic Field

$$H_{SOC} = \frac{1}{4mc^2}\boldsymbol{\sigma}\cdot\overbrace{gradV(x)\times p}^{\text{Effective Magnetic Field}}$$

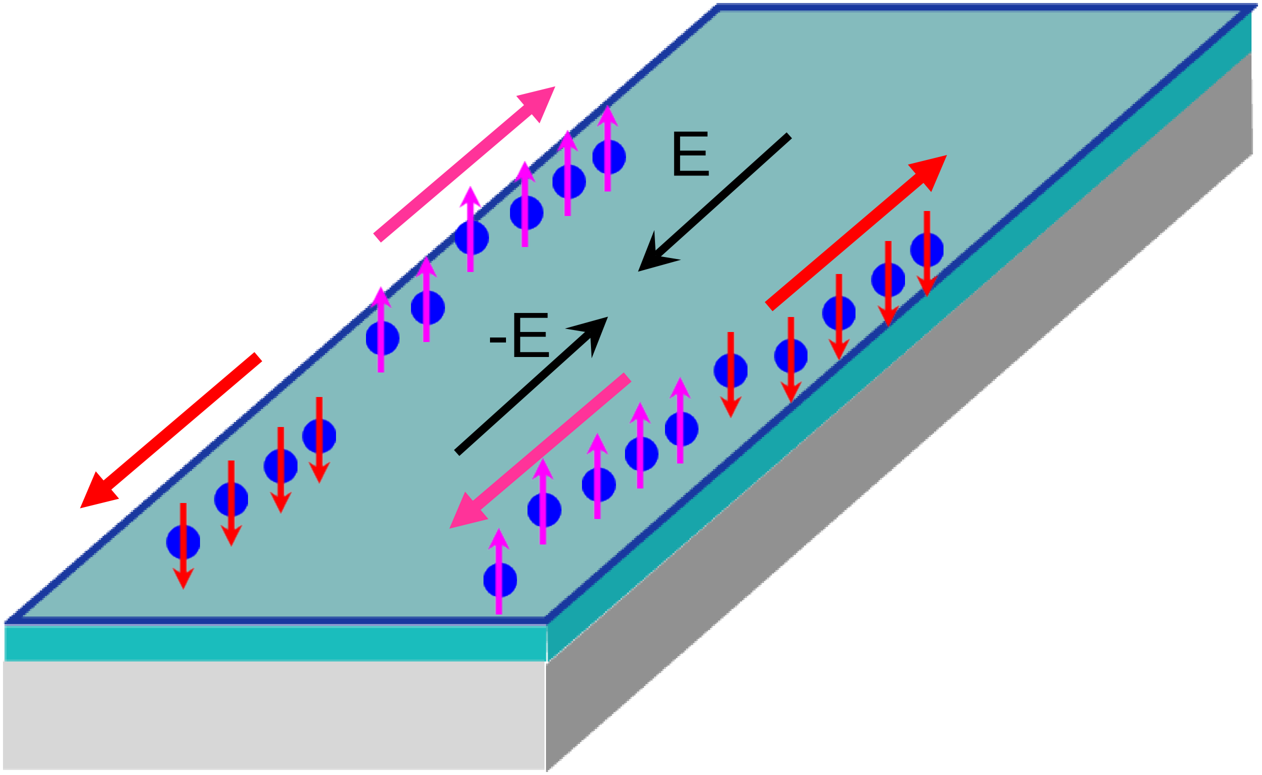
Spin Hall Effect

Spin flow at edges
⇒Spin accumulation
at edges
⇒chiral edge states



Surface states :
Spin-split due to
Rashba effect or
Topological insulators

Spin Current flowing at Edges



Quantum (Spin) Hall Sate Without Magnetic Field!

Spin-Orbit Interaction

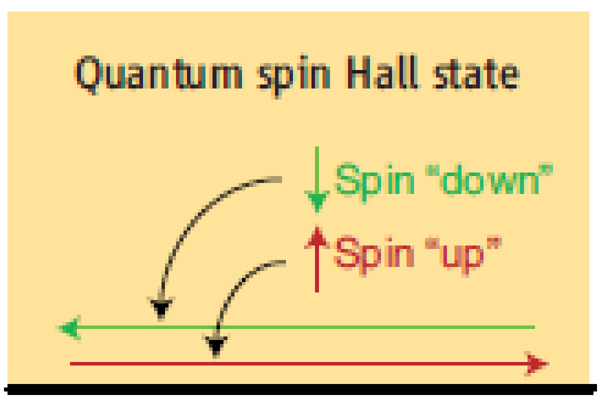
→ **Electric field = Effective magnetic field**

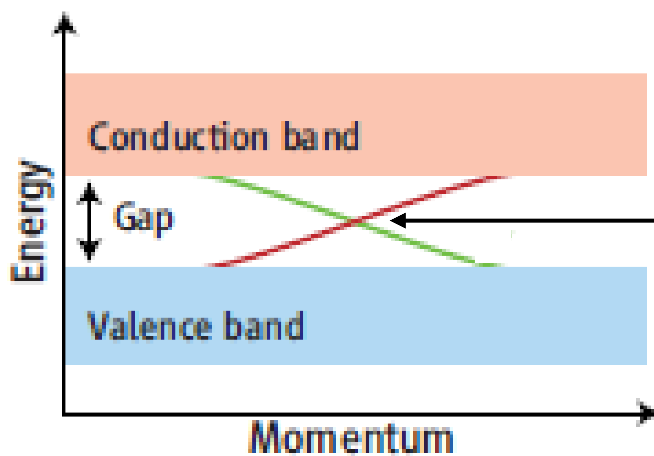
for moving electrons

→ { **Bulk; insulator**

Surface; **Spin-split metal (Kramers degeneracy is lifted)**

Spin flow

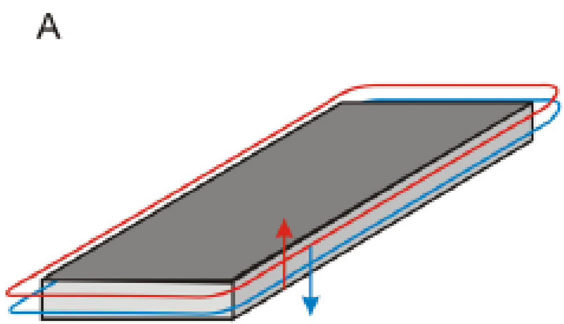




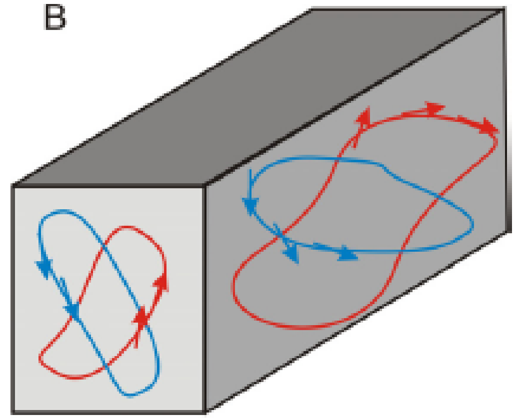
(Chiral) Dirac Fermion

Bulk; insulator
Surface; (Topologically protected)

Quantum spin Hall phases and topological insulators



2D QSH phase



3D topological insulators

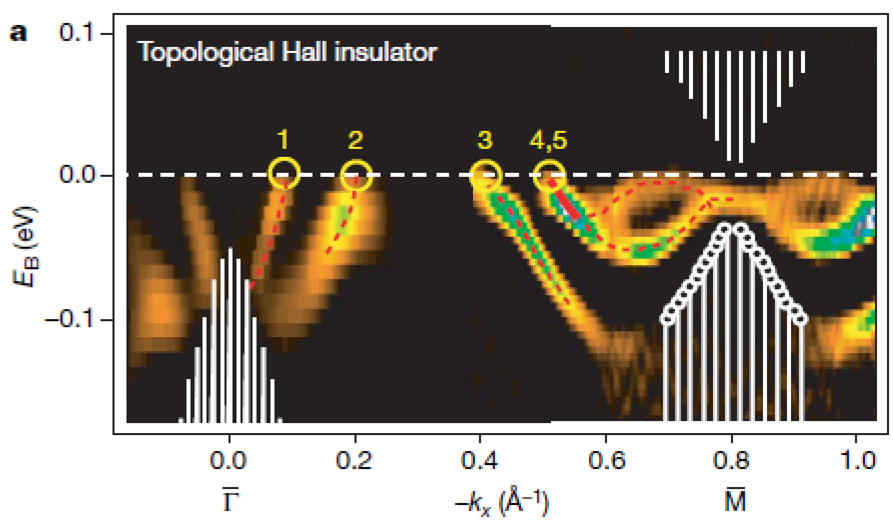
- bulk = gapped
- Gapless edge states

Spin-orbit coupling

- Carry spin current
- Robust against weak non-magnetic impurities or interaction (**topological metal**)

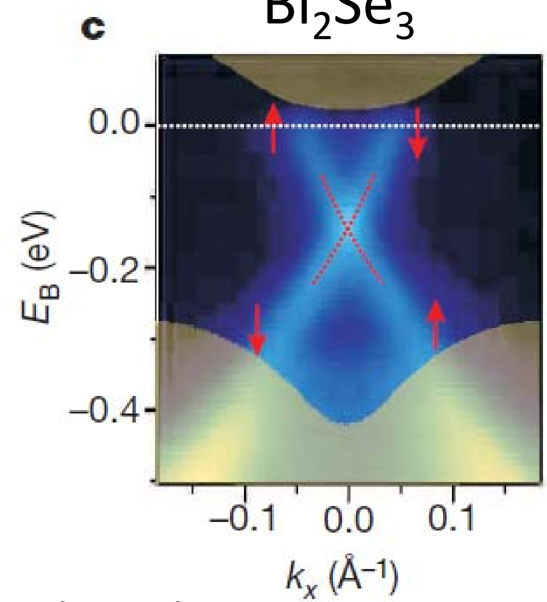
(S)ARPES

$Bi_{1-x}Sb_x$ $(0.07<x<0.22)$



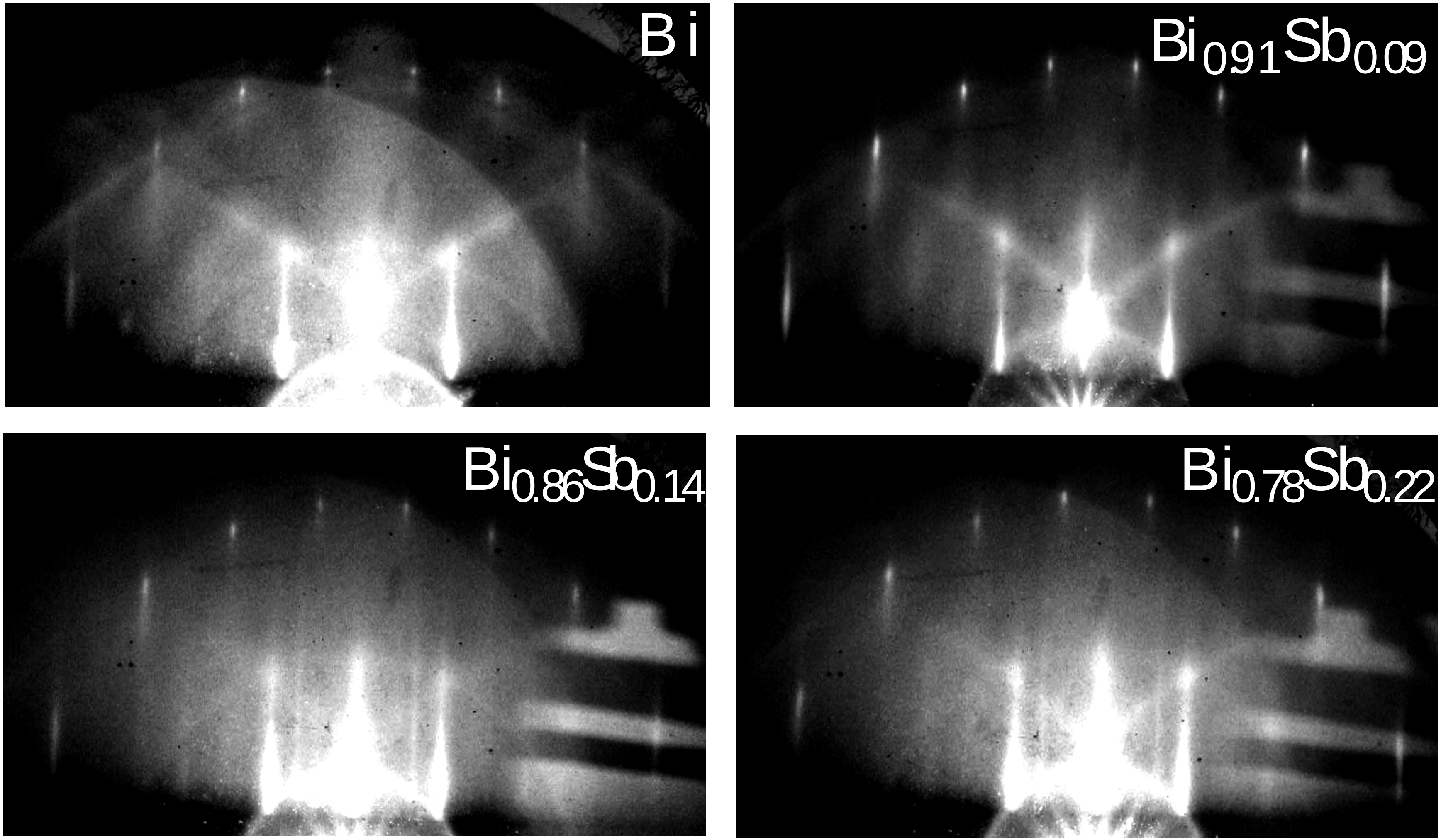
D. Hsieh *et al.*, Nature **454**, 970 (2008)

Bi_2Se_3



D. Hsieh *et al.*, Nature **470**, 1101 (2009)

Co-deposition of Bi & Sb on Si(111)-7x7 at RT: RHEED observation

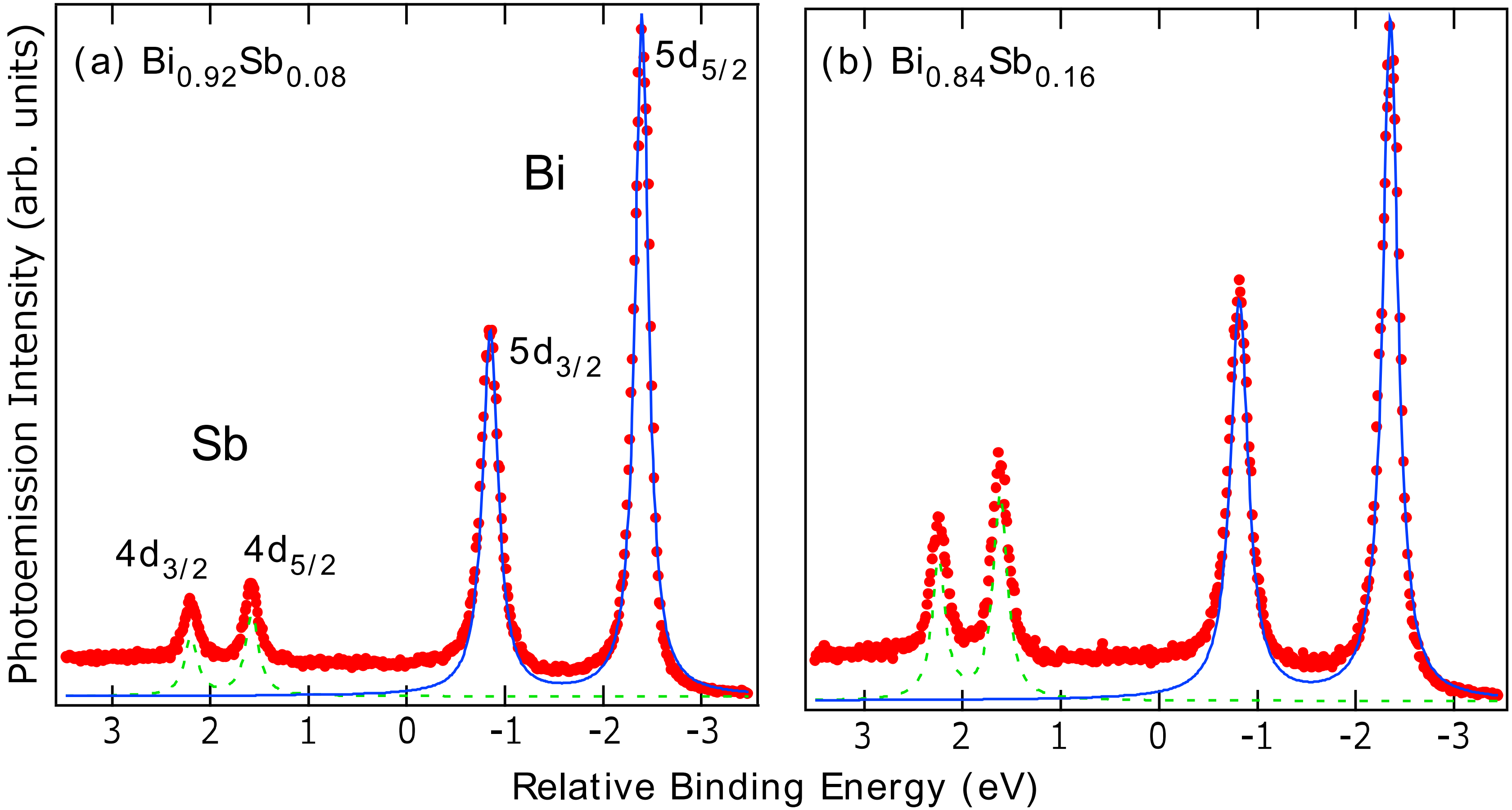


30 Å(7 BL) ultrathin film

- Sharp spots of 1x1 periodicity(001)
- Kikuchi pattern

Stoichiometry estimation by CLS

hν = 80 eV



$$\frac{\rho_{\mathrm{Bi}}}{\rho_{\mathrm{Sb}}} = \frac{I_{\mathrm{Bi}}}{S_{\mathrm{Bi}}} \Big/ \frac{I_{\mathrm{Sb}}}{S_{\mathrm{Sb}}} \sim 11.4$$ **(Sbが8.8%)**

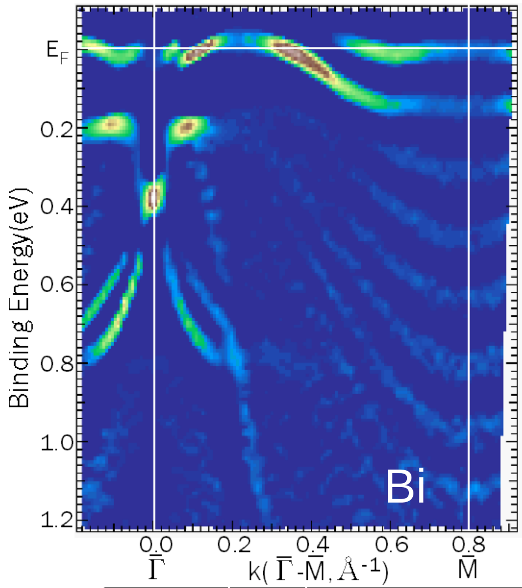
S_{Bi}: 11.07 S_{Sb}: 15.88

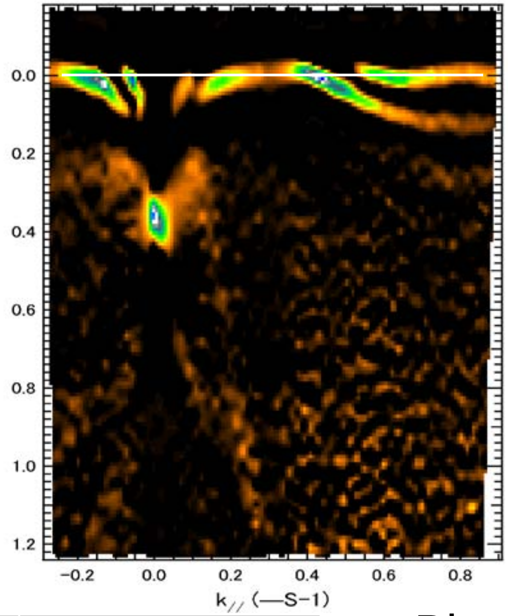
$$\frac{\rho_{\mathrm{Bi}}}{\rho_{\mathrm{Sb}}} \sim 5.4$$ **(Sbが18.5%)**

Good match!

J. Yeh and I. Lindau, At. Data Nucl. Data Tables 32, **1** (1985).

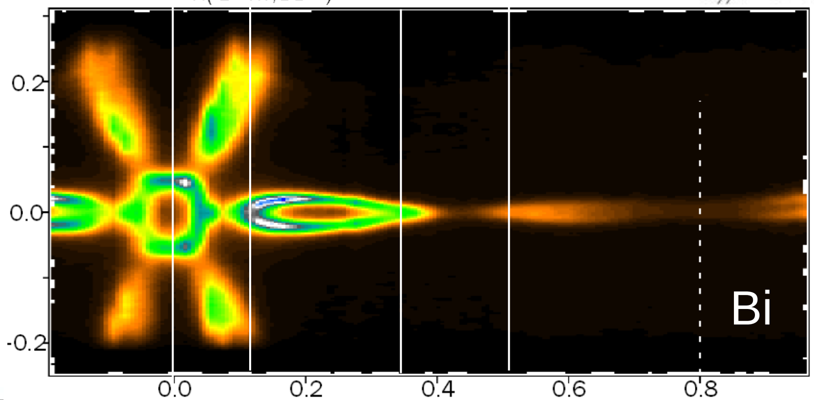
Comparison

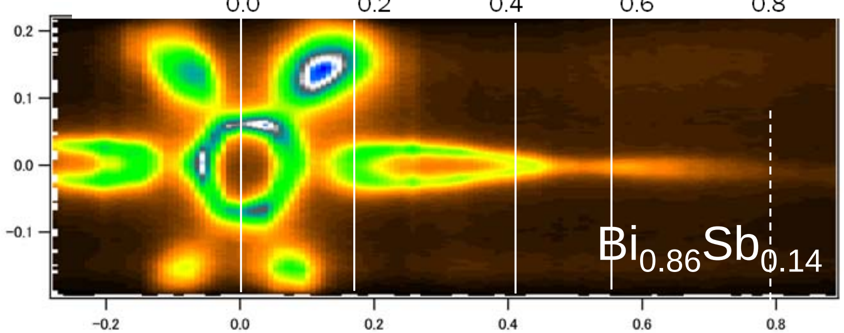




The surface states at E_F are almost the same between Bi and $Bi_{0.86}Sb_{0.14}$.

$Bi_{0.86}Sb_{0.14}$

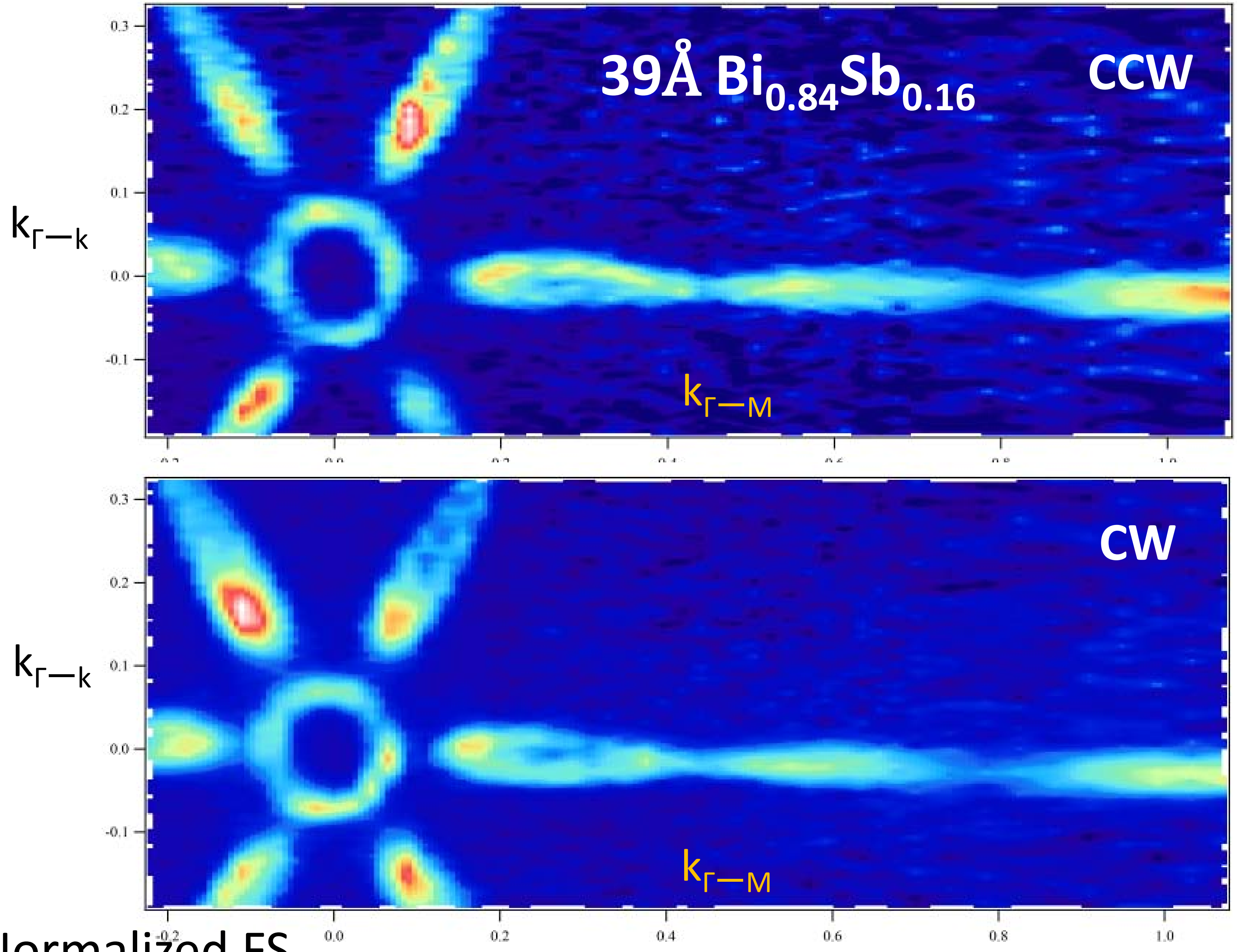




$Bi_{0.86}Sb_{0.14}$ and Bi

Band dispersion
Fermi Surface } Almost same

Helicity dependence - dichroism effect -



Normalized FS

Resistivity

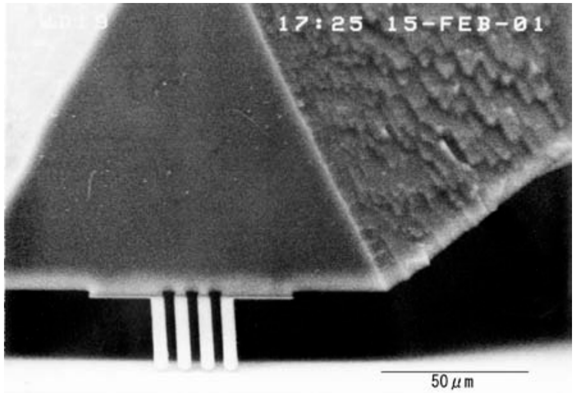
$Bi_{0.9}Sb_{0.1}$

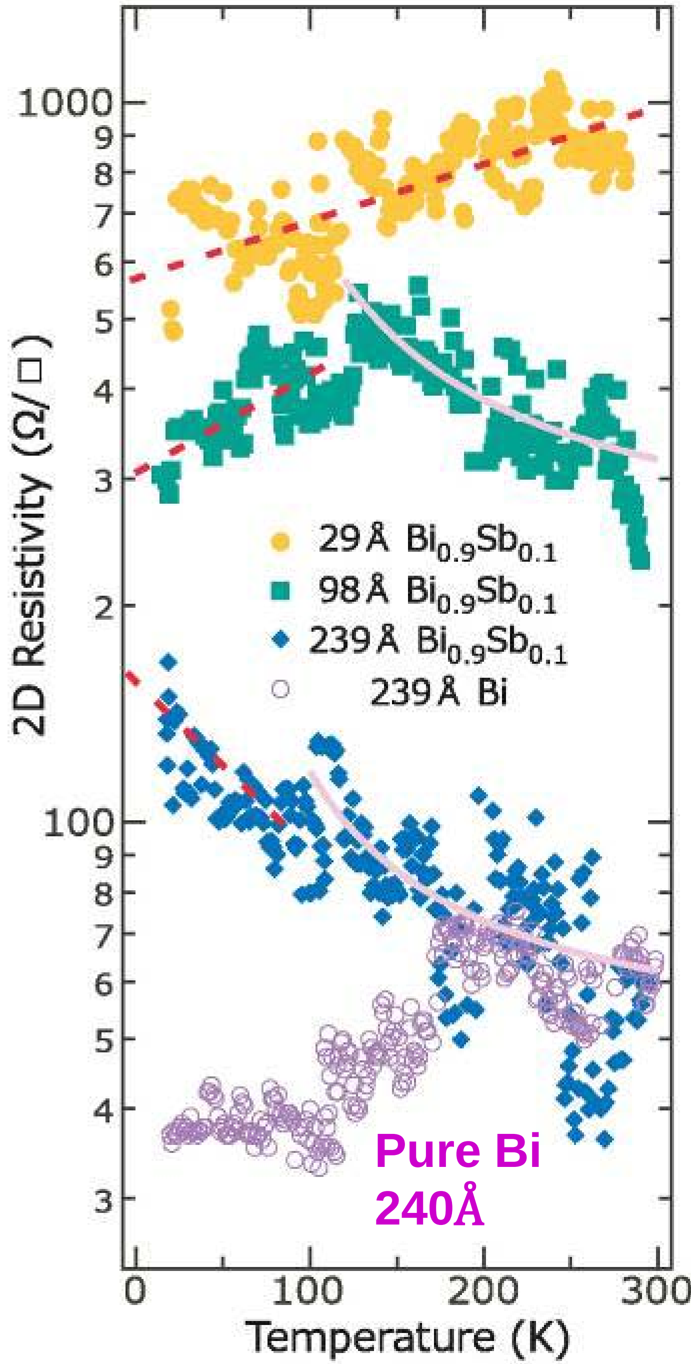
The surface is metallic, while bulk is insulating.

Bi

The surface is metallic, while bulk is (semi)metal.

In situ Micro-Four-Point Probe Measurement in UHV





$Bi_{0.9}Sb_{0.1}$

30Å

metallic

⇒Surface State

100Å

insulator-to-metal transition

240Å

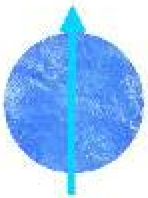
insulating

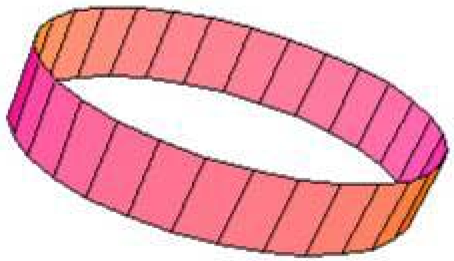
⇒Bulk State

T. Hirahara, et al, PRB**81**,165422 ('10).

2π-rotation of spin

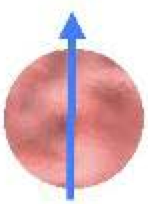
Spin=1

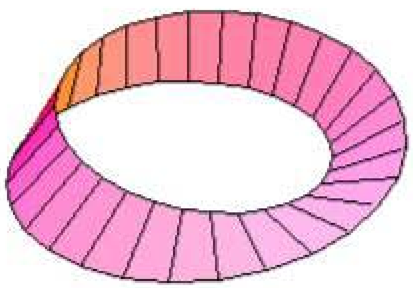




$\Psi \xrightarrow{2\pi\text{-rotation}} \Psi$

Spin=1/2



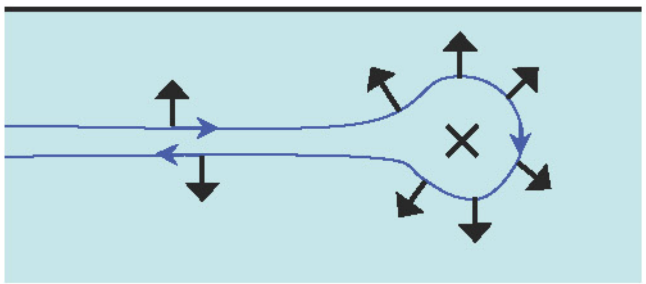


$\Psi \xrightarrow{2\pi\text{-rotation}} -\Psi$

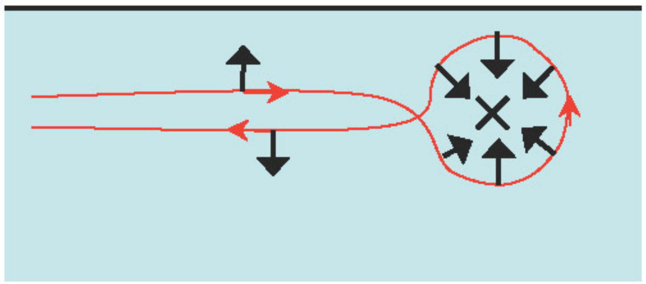
Spinor

Time-Reversal Symmetry

$E(k,\uparrow)=E(-k,\downarrow)$



$\Psi_{initial} \xrightarrow{\pi\text{-rotation}} \Psi_{scattered1}$



$\Psi_{initial} \xrightarrow{-\pi\text{-rotation}} \Psi_{scatter2}$

$\Psi_{scatter2} = -\Psi_{scatter1}$

$\Psi_{scatter1} + \Psi_{scatter2} = 0$

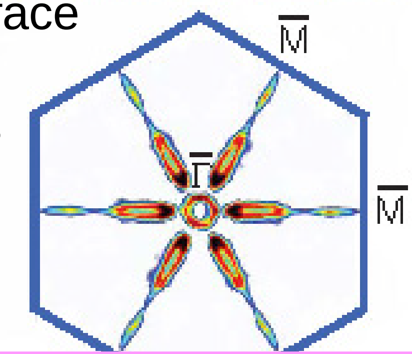
Destructive interference ⇒ **No backscattering**

Topological surface states protected from back scattering by chiral spin texture

Yazdani Group, Nature **460**, 1106 (2009)

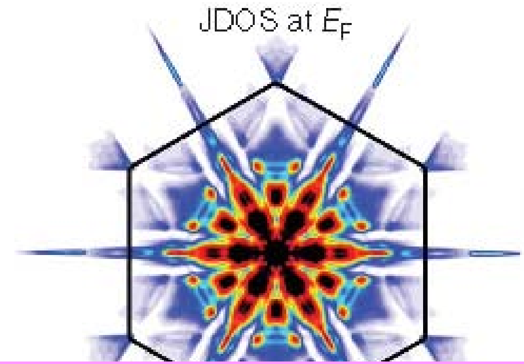
Fermi Surface mapped by ARPES

$I(k)$

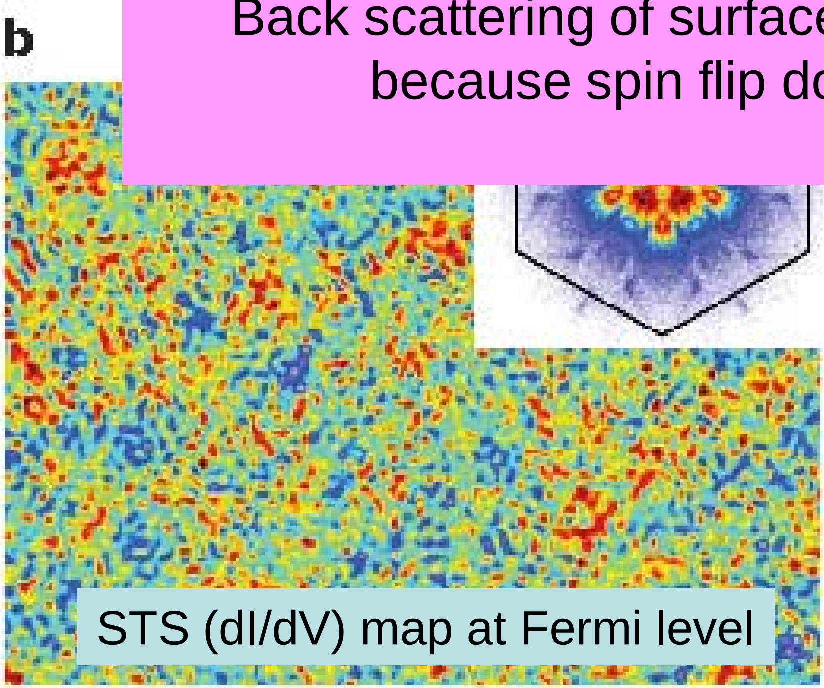


calculate

$JDOS(q)$



Back scattering of surface-state electrons are suppressed because spin flip does not occur at scattering.



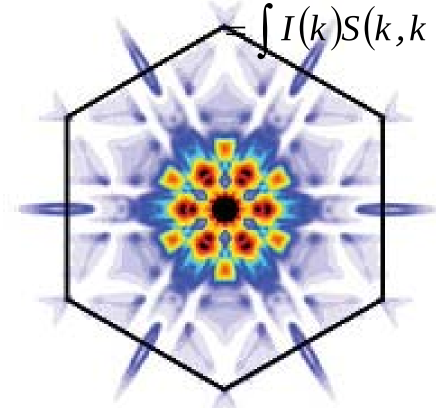
FT pattern

Good match

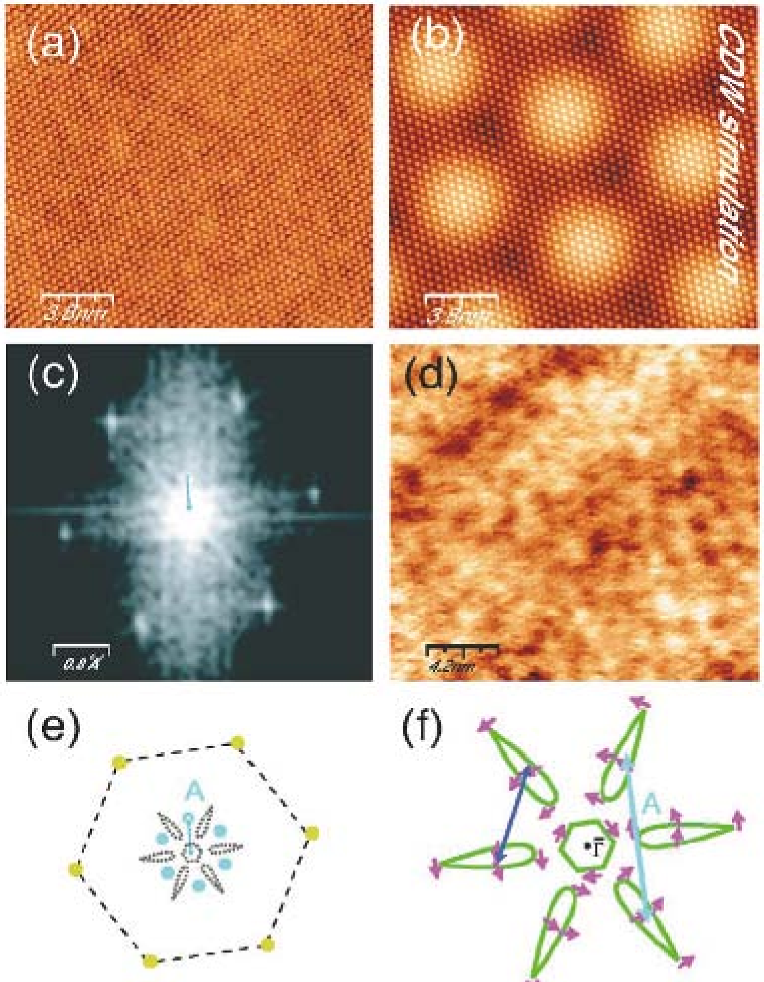
c

$SJDOS(q)$

$= \int I(k) S(k, k+q) I(k+q) d^2k$

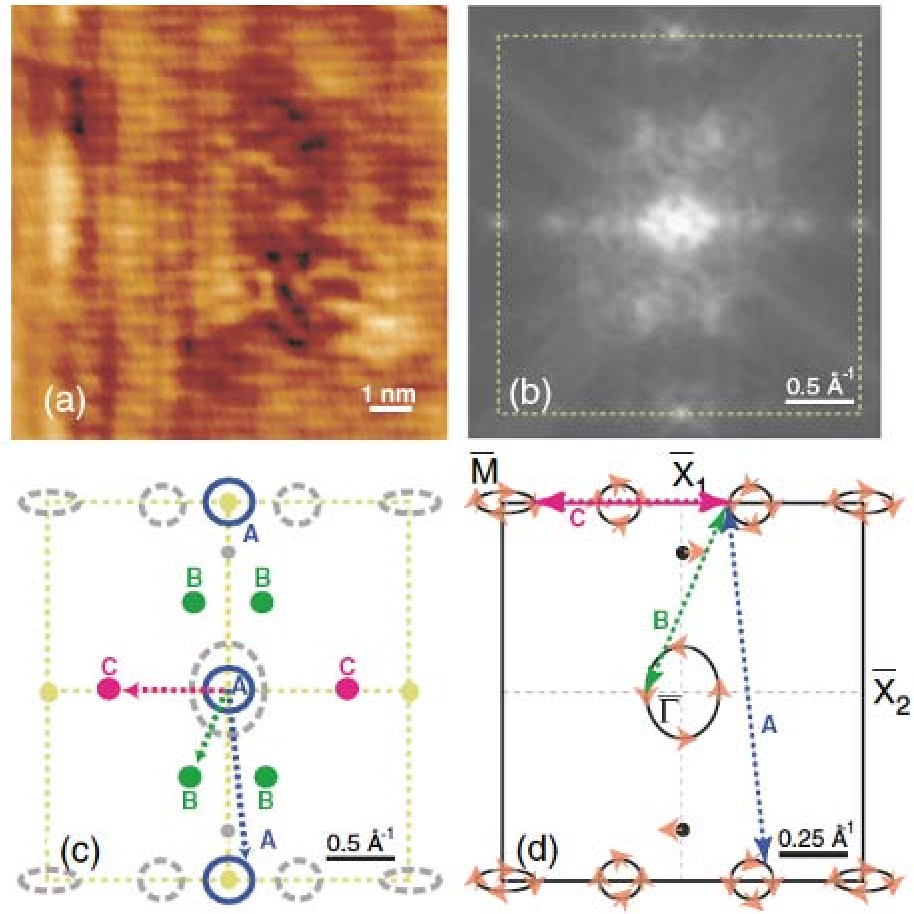


Role of spin in quasiparticle interference on Bi Surface



Bi(111)

T. K. Kim *et al.*, PRB **72**, 085440(2005).



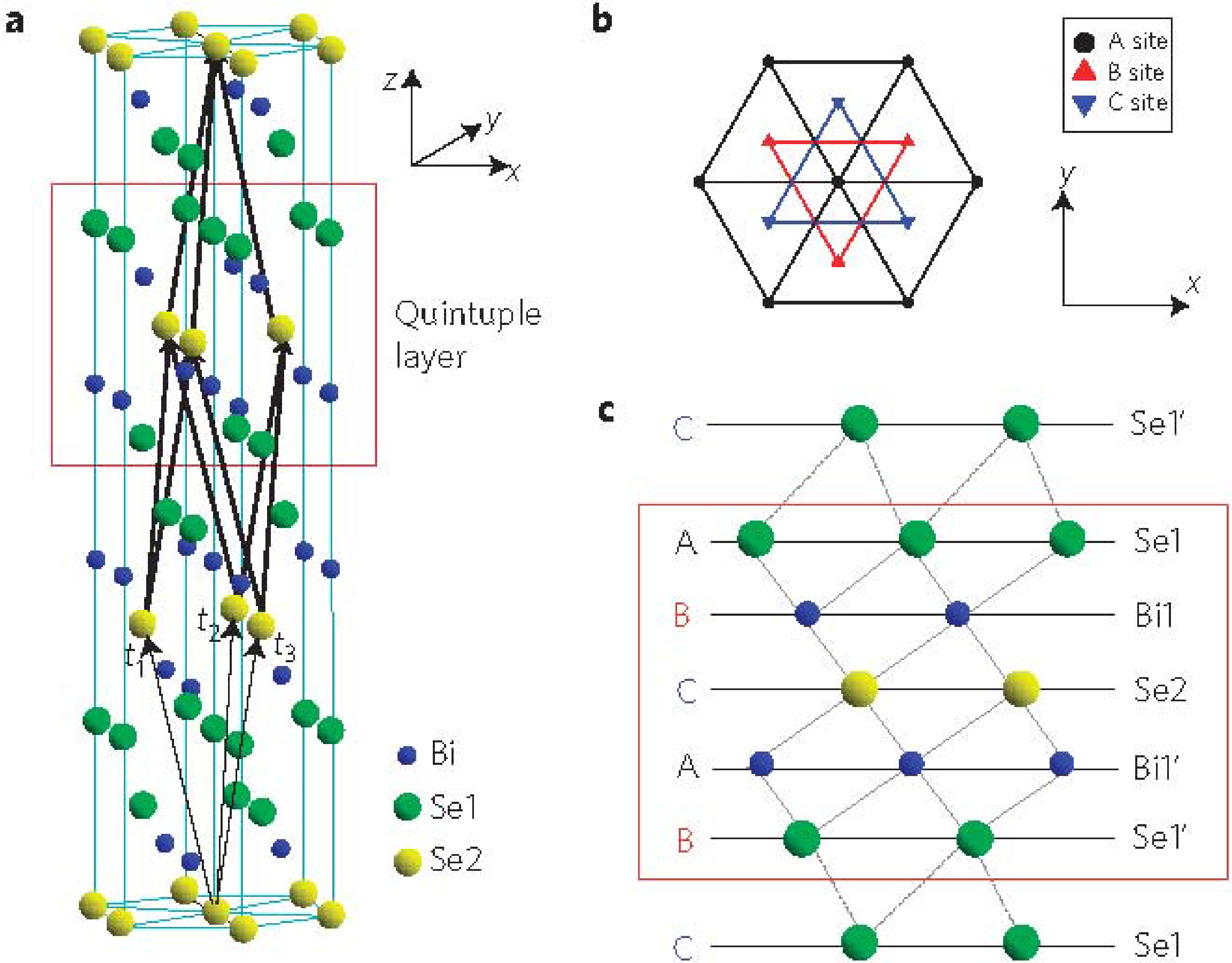
Bi(110)

J. I. Pascual *et al.*, PRL **93**, 196802(2004).

Spin-conserving scattering process \

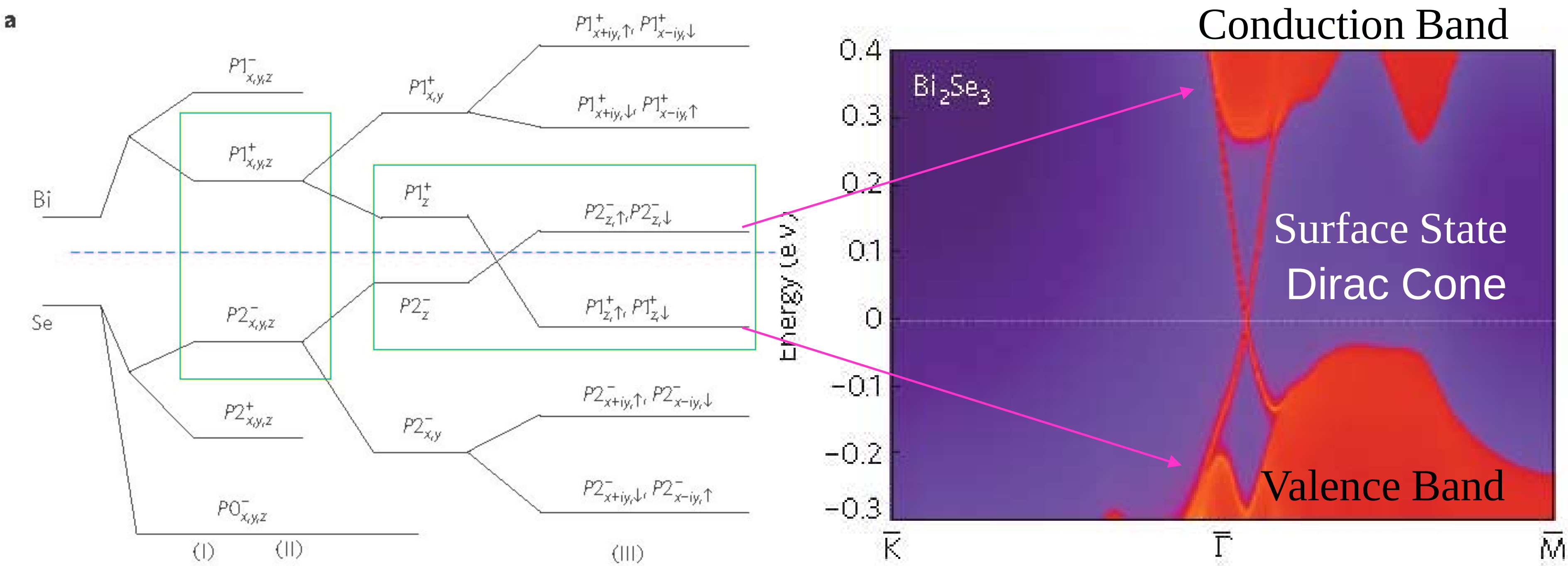
Crystal Structure of Bi_2Se_3

H. Zhang, et al., Nature Physics (May 2009)



Electronic Structure of Bi_2Se_3 （Theory）

H. Zhang, et al., Nature Physics (May 2009)



Isolated Atoms （Atomic Orbital）

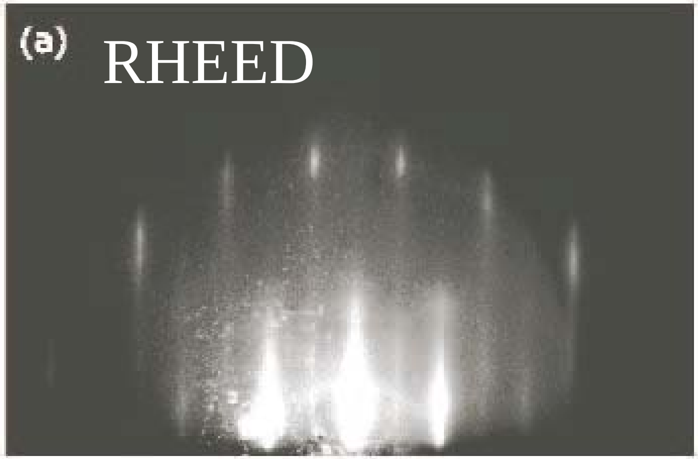
Atomic Bondings

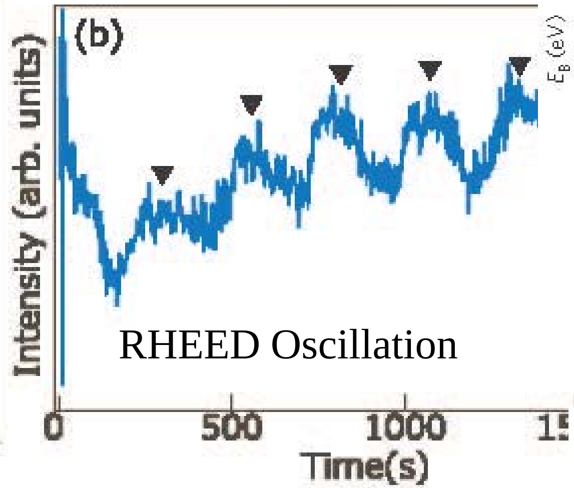
Split due to Crystal Field

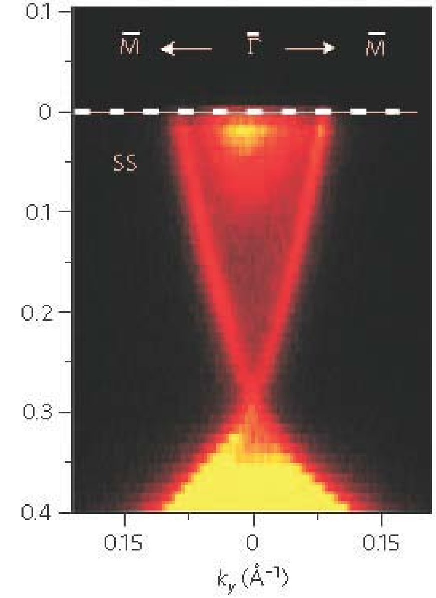
Spin-Orbit Intercation

Growth and Band Structure of Bi_2Se_3

Y. Sakamoto, et al., Phys. Rev. B**81**,165432 (2010)







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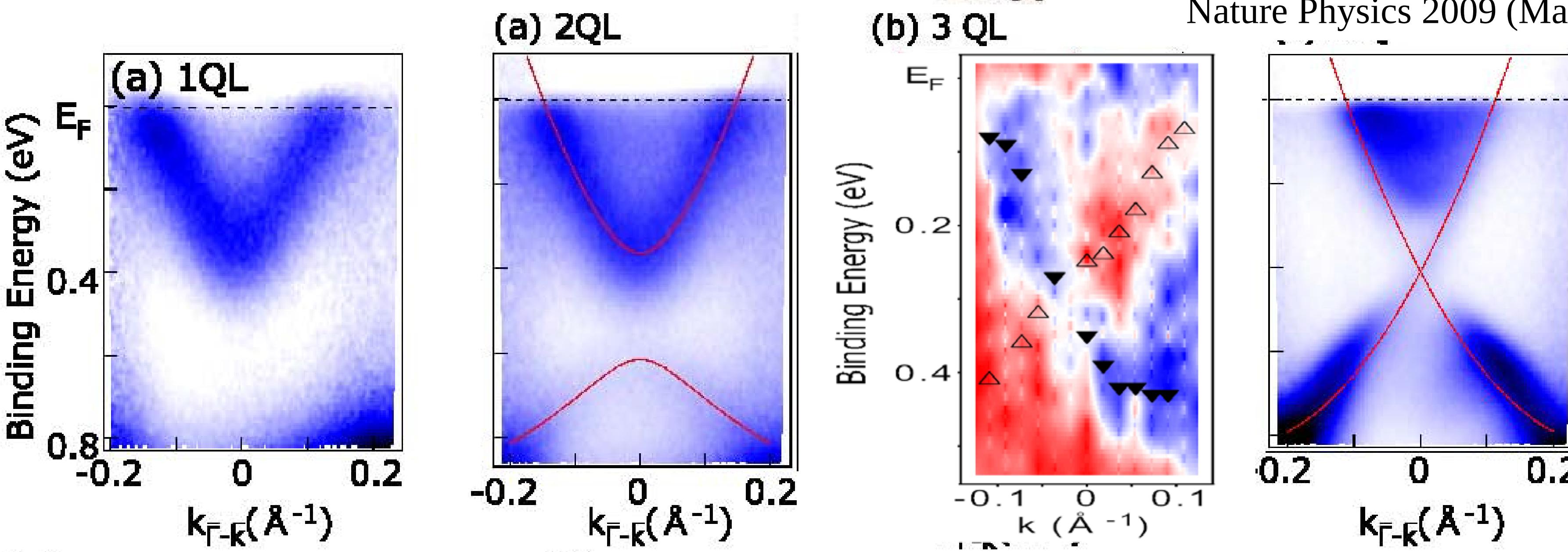
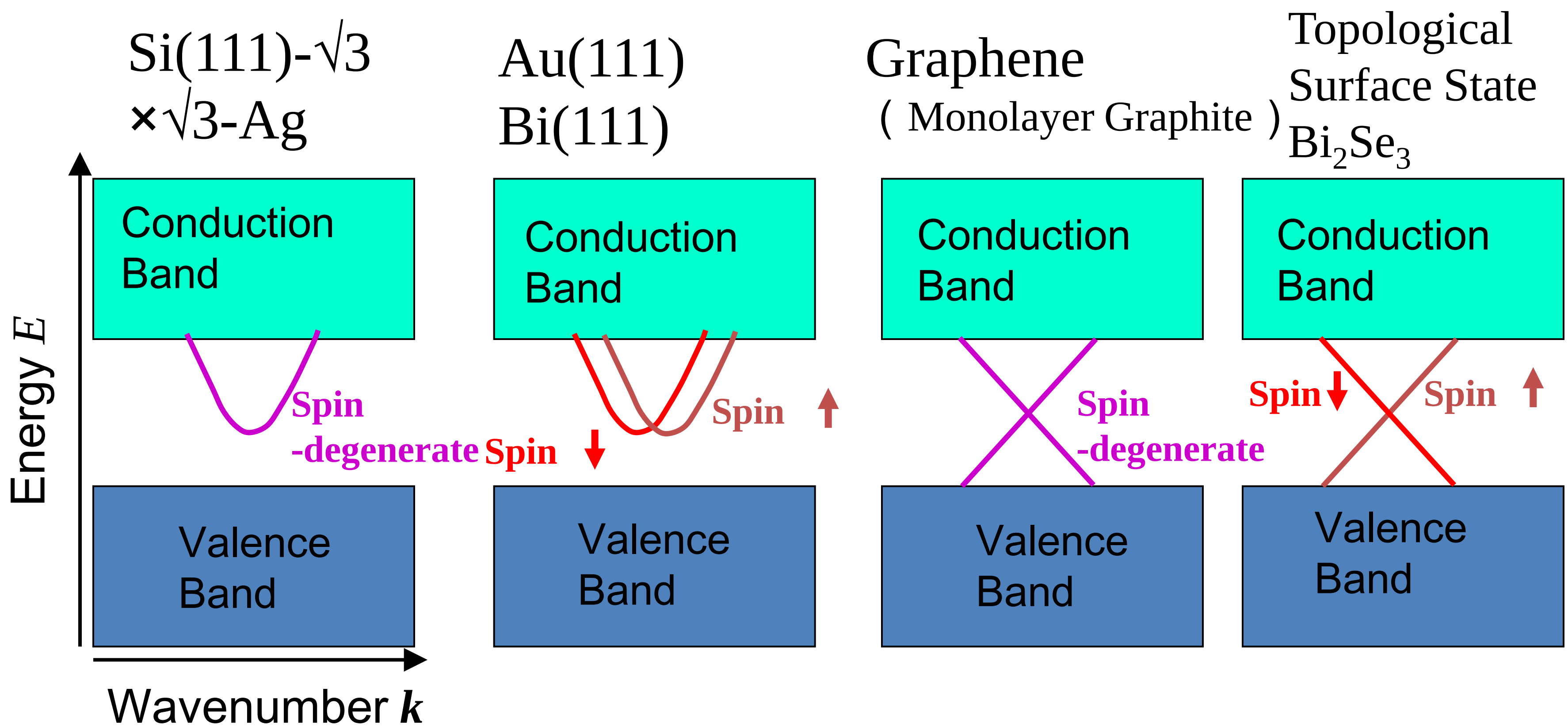
vth

Bulk Crystal Y. Xia, et al., Nature Physics 2009 (May)



Various Surface Sates



$$E = \frac{p^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*}$$

Free-Electron-like

$$E = \sqrt{(mc^2)^2 + (pc)^2}$$

$$m = 0$$

$$E = \pm pc = \pm c\hbar k$$

Massless Dirac Fermion

Summary: Compare $Bi_{1-x}Sb_x$, Bi_2Se_3 with Bi

Both of $Bi_{1-x}Sb_x$ and Bi show

1. metallic spin-split surface state
2. chiral spin texture in Fermi surface
3. absence of back scattering in surface state

   ⇒ These are not unique properties of topological insulators.
   Surface Rashba effect bring about them.

4. Chiral Dirac cone in surface state: Bi_2Se_3

The unique properties of topological insulators may be detected in Spin flow.

Spin Transport Measurements

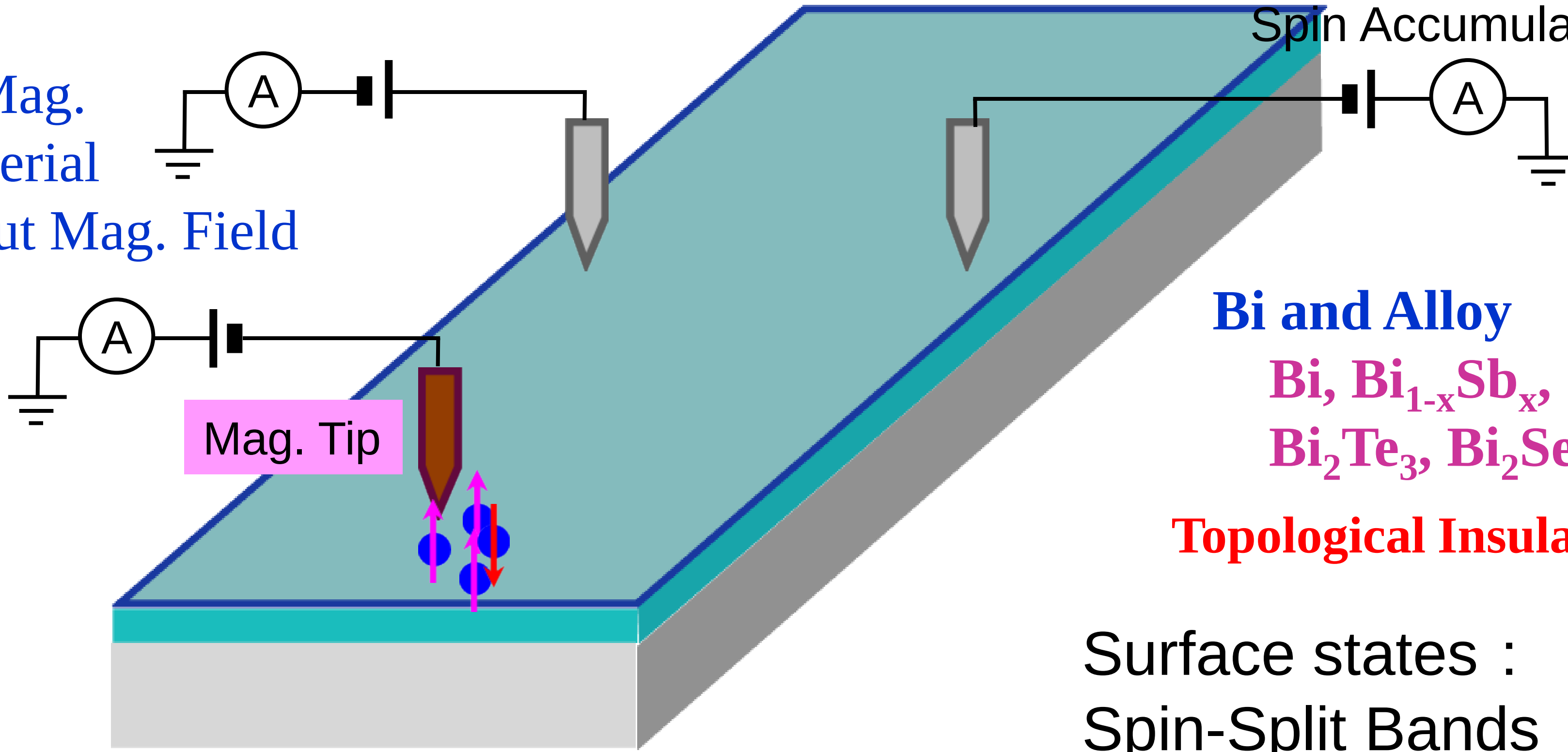
Strong Spin-Orbit Interaction

⇒Electric field is seen to be effect magnetic field for flowing electrons

⇒Spin flow perpendicular to Current and spin : Spin Accumulation

3 -tip STM

Non-Mag. Material Without Mag. Field



Bi and Alloy

Bi, $Bi_{1-x}Sb_x$, Bi_2Te_3, Bi_2Se_3

Topological Insulator

Tip Separation < Spin Relaxation Length

Surface states :
Spin-Split Bands
Due to Rashba Eff.

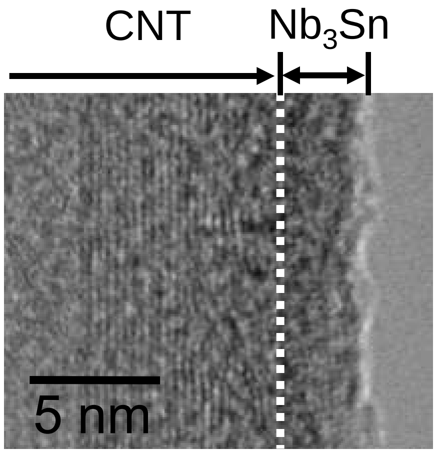
$$H = \frac{1}{2m} p^2 + V(x) + \frac{1}{4mc^2} \sigma \cdot \left(gradV(x) \times p \right)$$

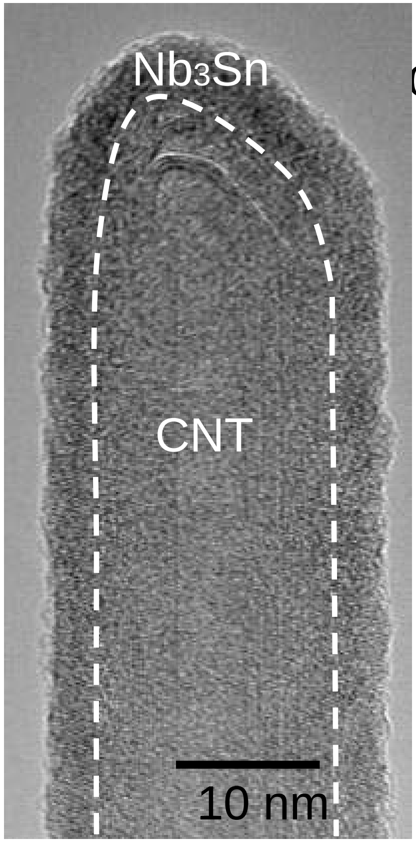
Functionalized CNT Tips with Coating

Coating CNT Tips with Compounds and Multi-Layers
→ Various Measurements

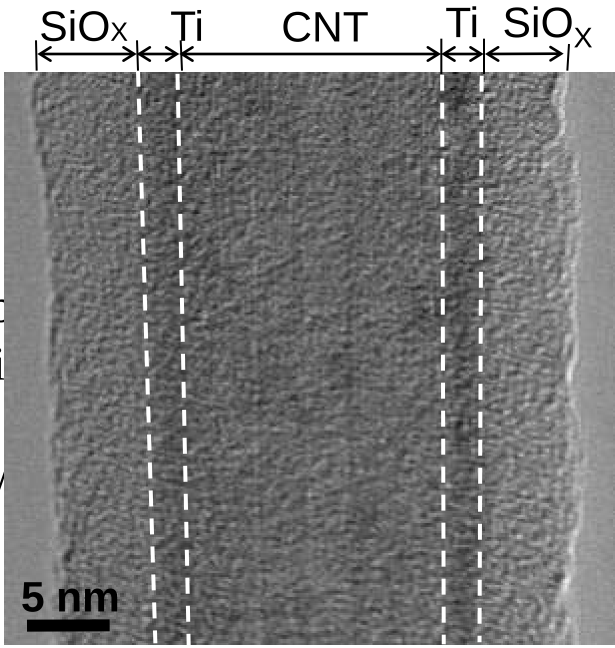
- Metal → Ohmic or Schottky Contacts W, PtIr
- Dielectric (Insulator) → Nano-FET effect SiO_2
- Magnetic → Spintronics、MFM CoFe
- Superconducting → Andreev Ref.、SC devices Nb_3Sn, Nb
- Insulator/Metal Multi-Layers → STM in liquid、Biochemi

Probes

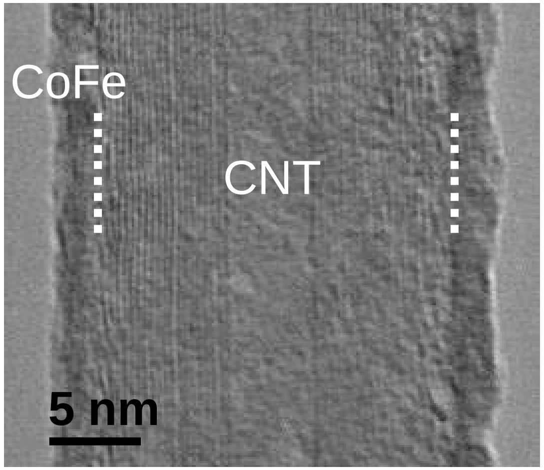




Ox/



CoFe

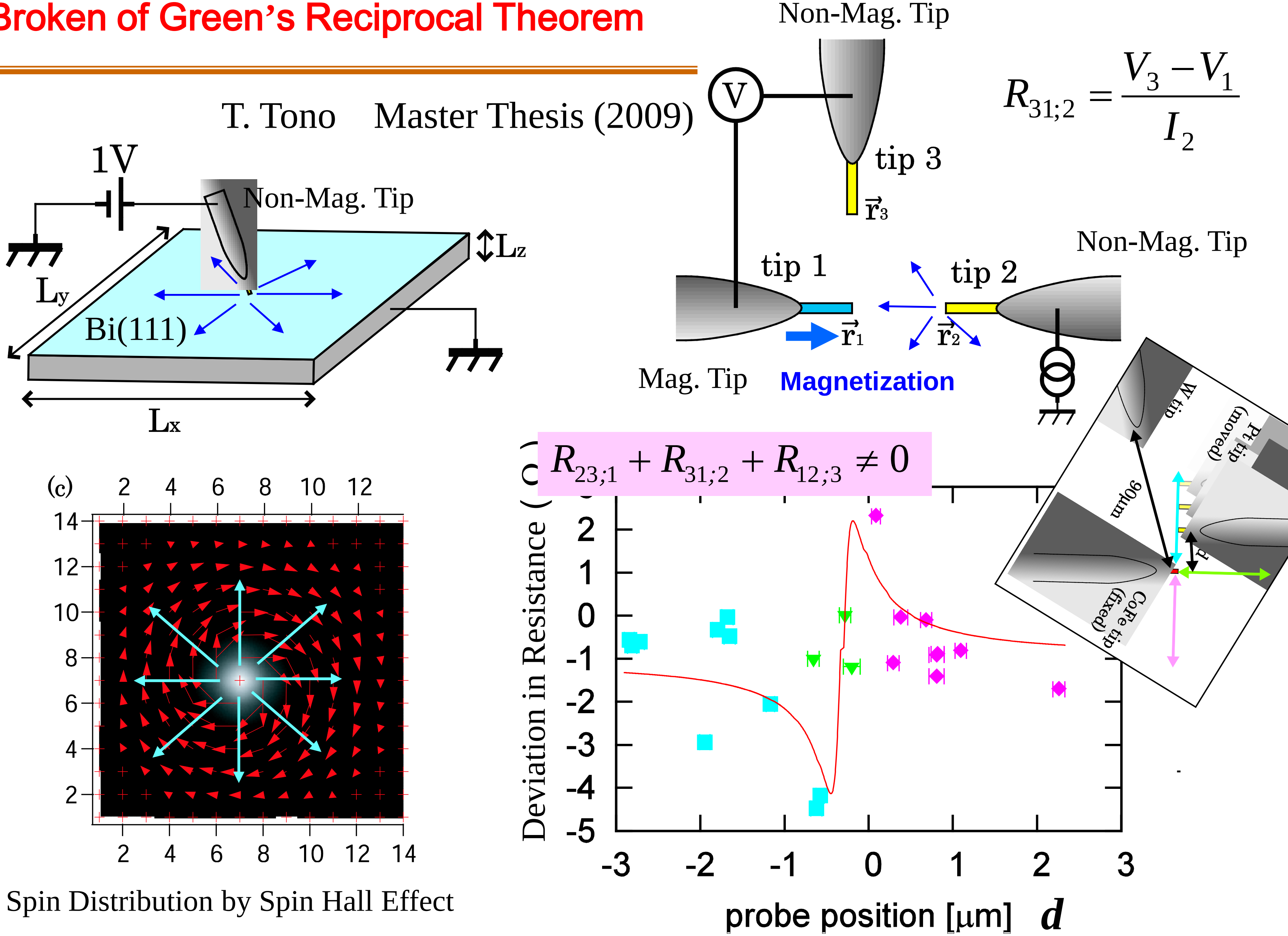


CNT Coating by Pulsed Laser Deposition （PLD）

H. Konishi, et al., JJAP 45, 3690 (‘06)
H. Konishi, et al., RSI 78, 013703(‘07)

Inverse Spin Hall Effect+Mag. Tip
⇒ Broken of Green's Reciprocal Theorem

T. Tono Master Thesis (2009)



Spin Distribution by Spin Hall Effect