

トポロジカル物質とは何か

—表面物理学の観点から—



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大学院理学系研究科物理学専攻

1. 表面電子状態
2. スピン分裂した表面電子状態
3. トポロジカル表面電子状態
4. 電子の位相
5. トポロジカル物質ファミリー

ブルーボックス
2021年1月21日出版



The Surface is Cool.



表面電子状態とは

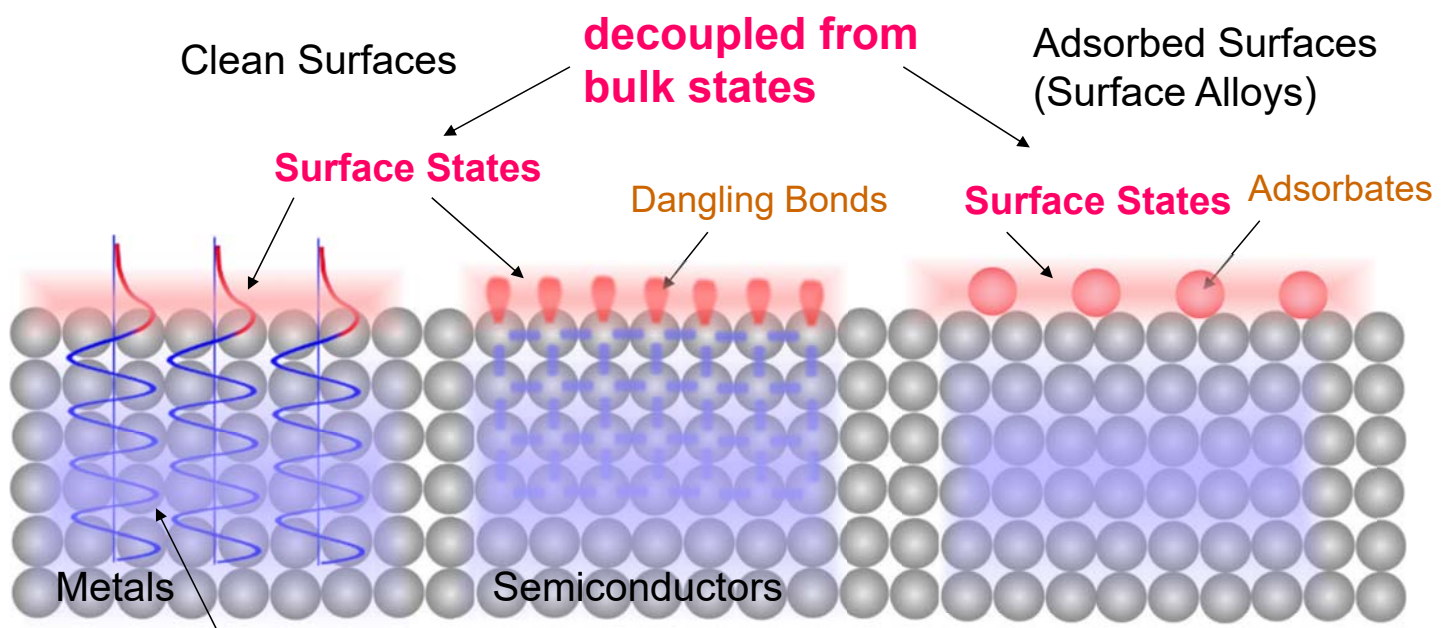
(1) 成因

(2) エネルギー

(3) 分散

Surface States — Shockley & Tamm States —

Chemical bonding and Potential at Surfaces



-Low-D Electronic Systems
-New Periodicity
-Broken (Space-Inv.) Symmetry

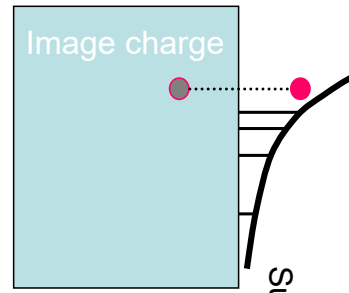
⇔ Topological surface states

表面 (電子) 狀態

1. Shockley states (extended)

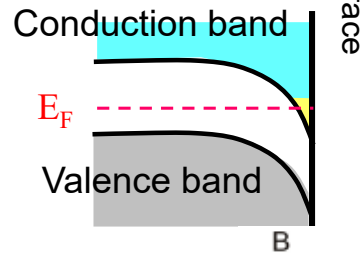
Tamm states (localized)

Chemical bonding,
Surface Potential



2. Image states

Image charge



3. Surface space-charge layer

Bending of bulk bands

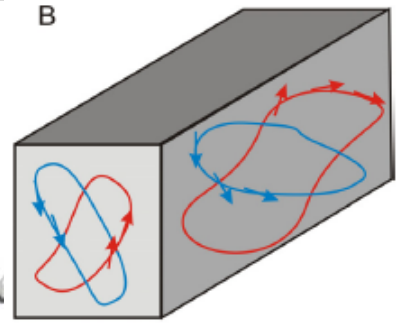
表面空間電荷層

4. Topological surface states

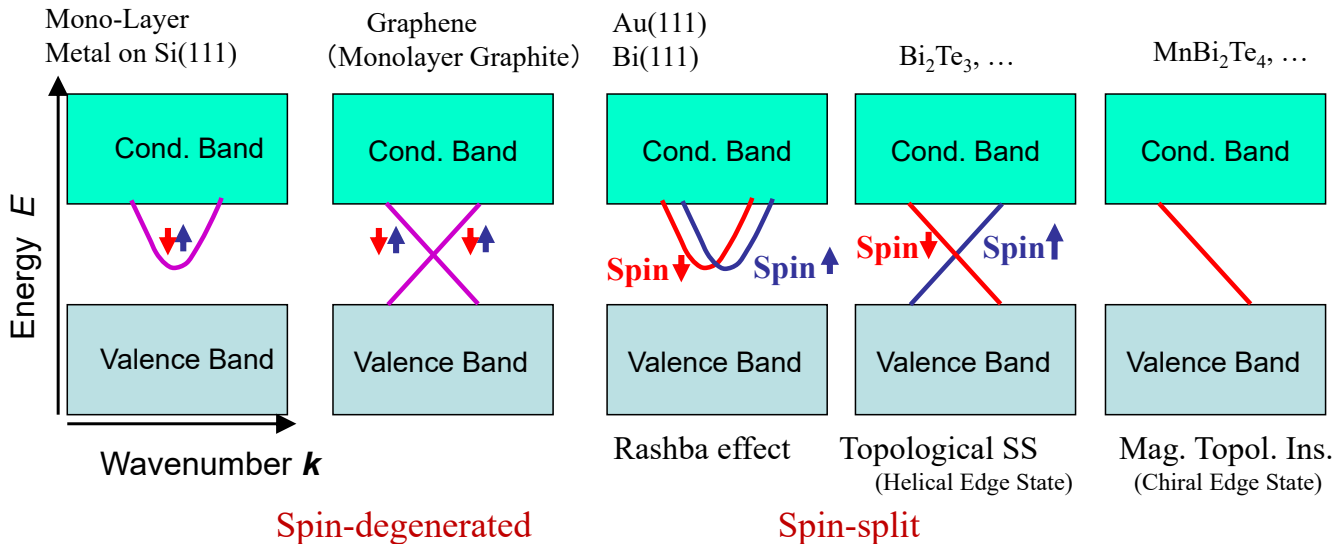
Quantum Hall Effect

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

HgTe (QW), Bi_{1-x}Sb_x, Bi₂Te₃, Bi₂Se₃,



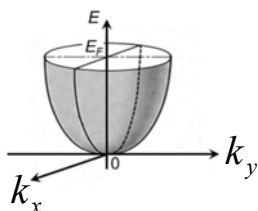
Various Surface States



Free-Electron-like States

(Non-relativistic)

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



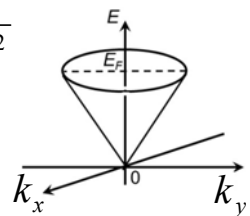
(Relativistic)

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

$$\Downarrow m = 0$$

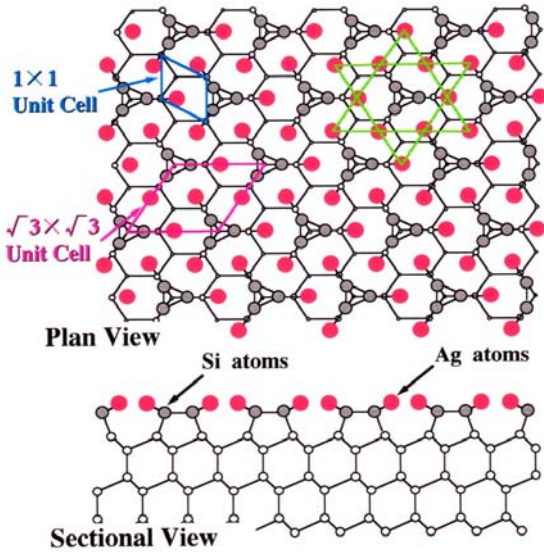
$$E = \pm pc = \pm \hbar ck$$

Massless Dirac Electrons



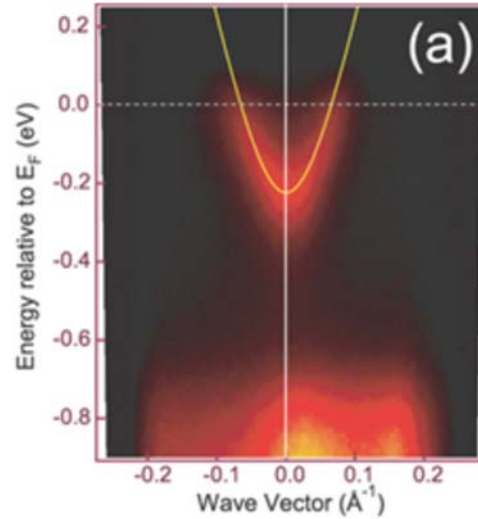
Mono-Layer Ag on Si : Si (111)- $\sqrt{3} \times \sqrt{3}$ -Ag Surface

2D Metal (Monatomic-Layer Metal)



- Inert and atomically flat surface
- Free-electron-like surface state

H. Aizawa, *et al.*, Surf. Sci. **429** (1999) L509
 T. Hirahara, *et al.*, Surf. Sci. **563** (2004) 191
 C. Liu, *et al.*, Phys. Rev. Lett. **96**, 036803 (2006)



$$E = \frac{p_{//}^2}{2m^*} = \frac{\hbar^2 k_{//}^2}{2m^*}$$

Parabolic Dispersion:
Free-Electron-Like State

Graphene on SiC crystal surface

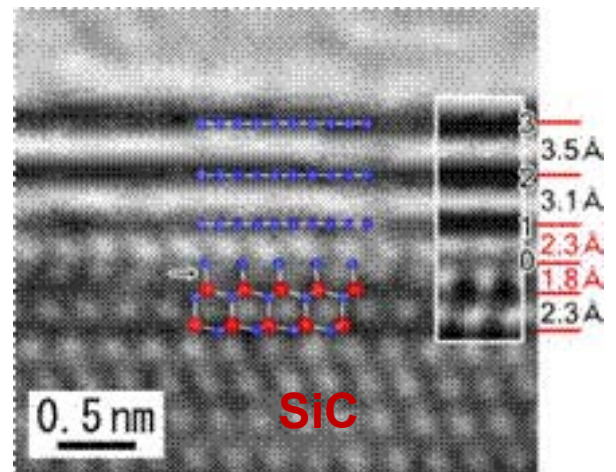
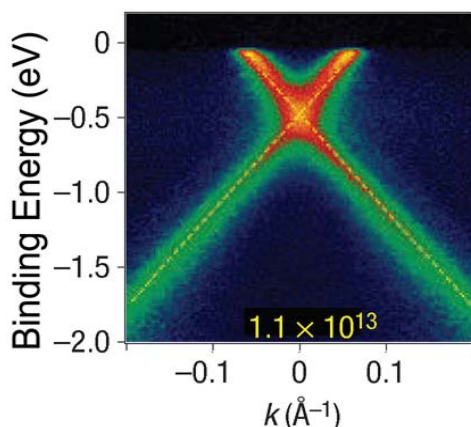
Relativistic Dirac electron

$$E = \sqrt{(mc^2)^2 + (c\hbar k)^2}$$

$m = 0$ Zero Mass

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

High mobility



(M. Kusunoki @ Nagoya U.)

Non-relativistic

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

スピン分裂した表面電子状態

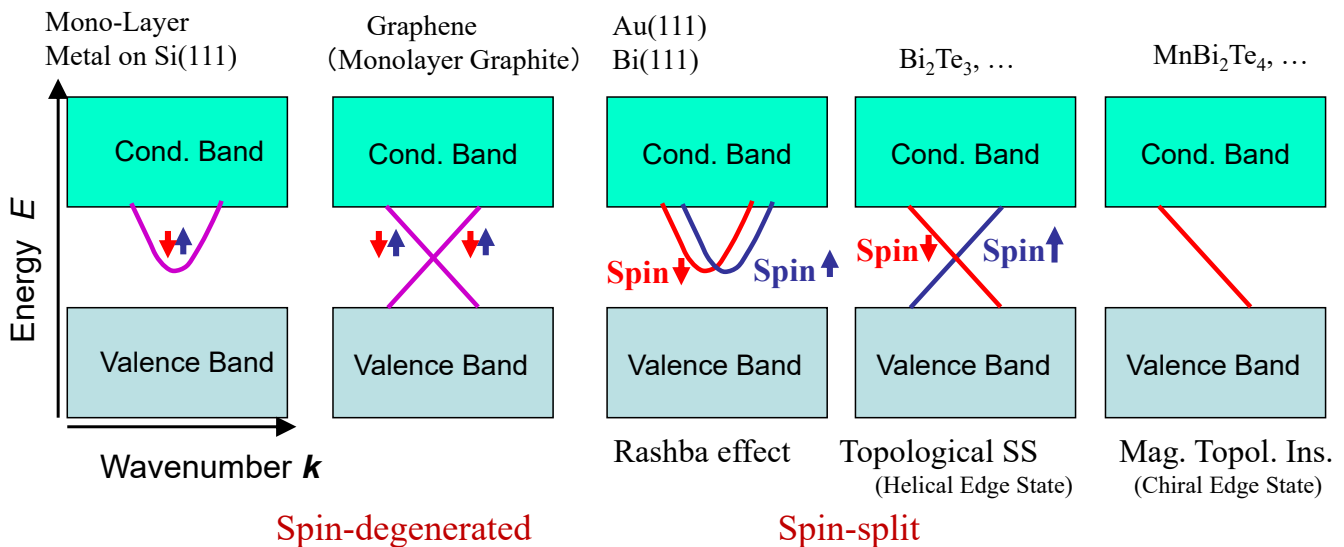
(1) 空間反転対称性の破れ

(2) スピン軌道相互作用

⇒ 仮想磁場

(3) ラッシュバ効果

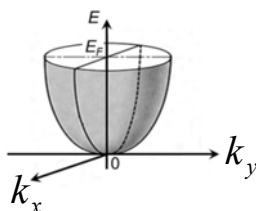
Various Surface States



Free-Electron-like States

(Non-relativistic)

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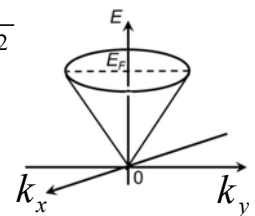
(Relativistic)

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

$$\Downarrow m = 0$$

$$E = \pm pc = \pm \hbar ck$$

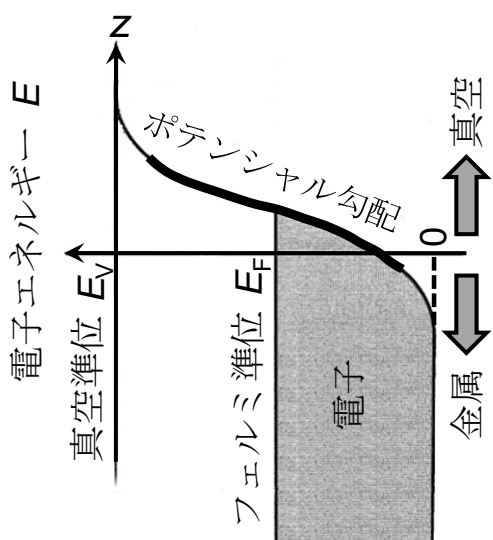
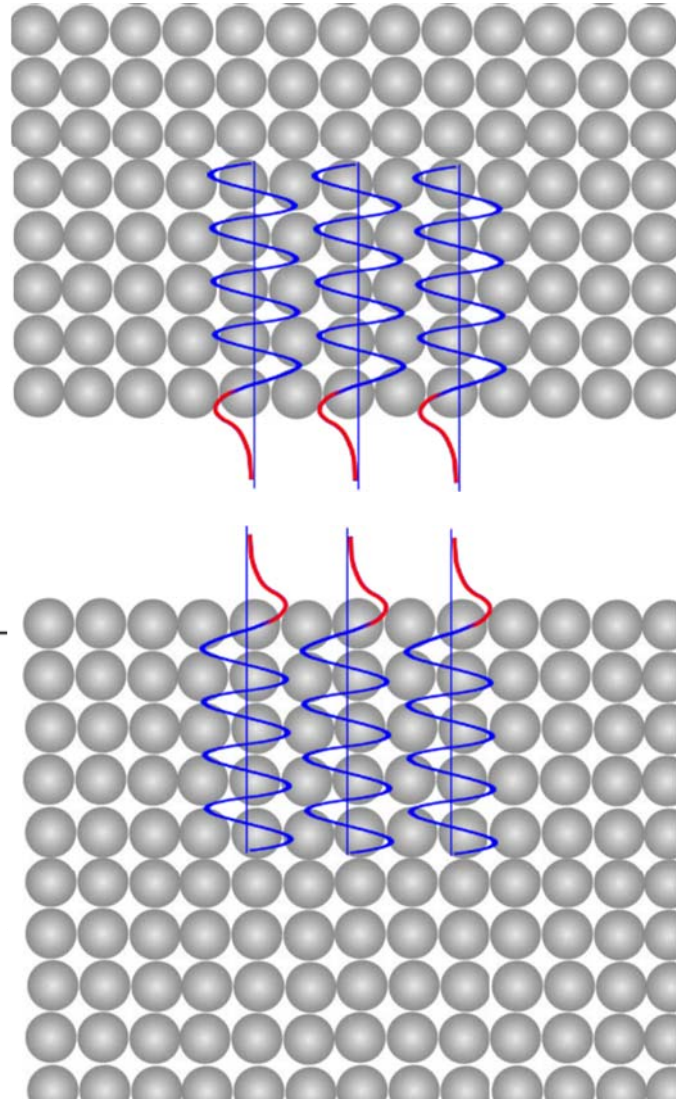
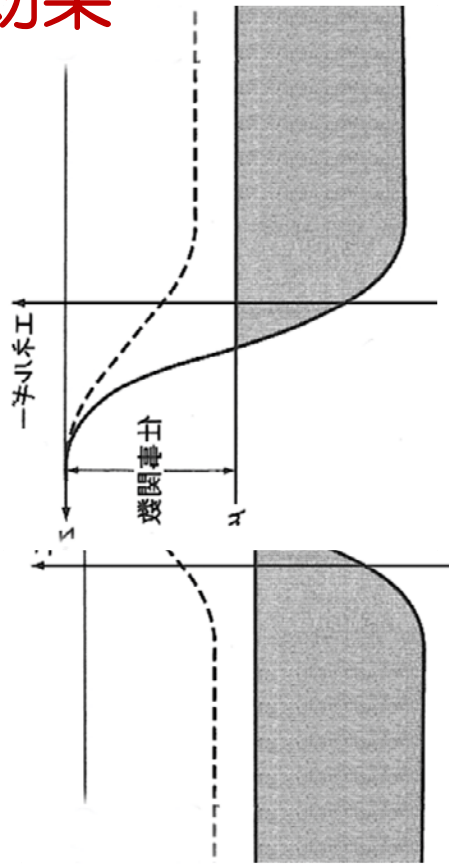
Massless Dirac Electrons



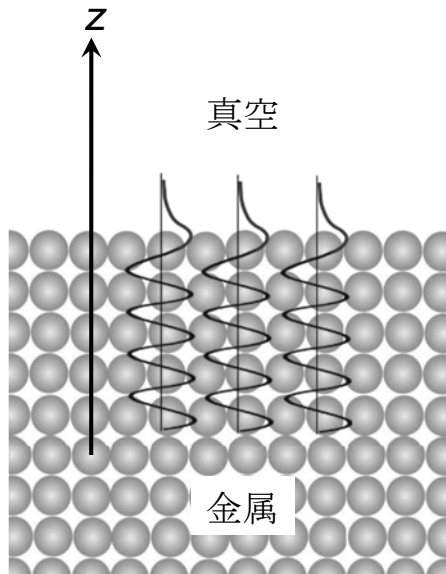
Rashba 効果



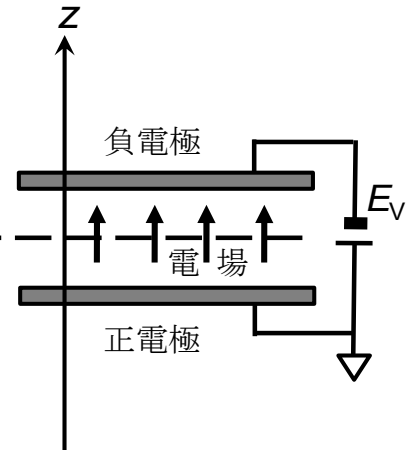
Emmanuel I. Rashba



(a) 結晶表面近くのポテンシャル

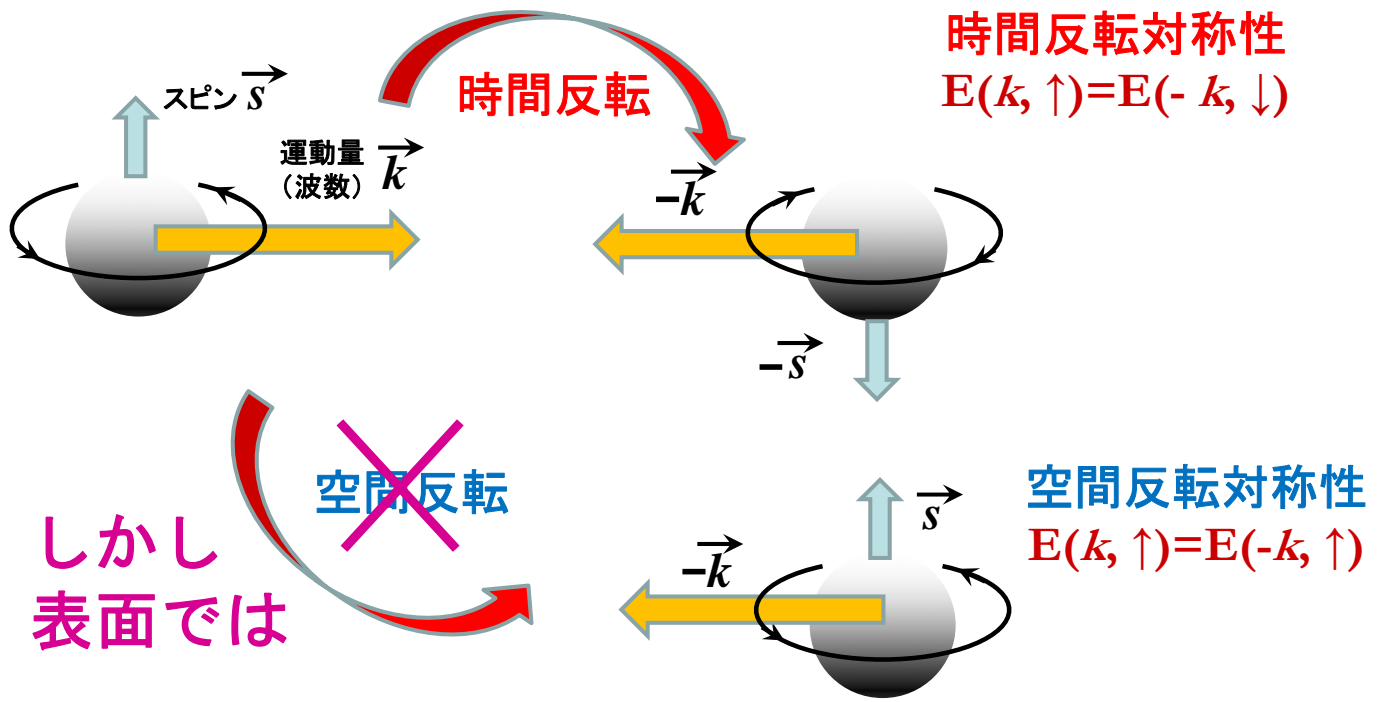


(b) 結晶表面近くの断面図



(c) 結晶表面近くの電場

電子のエネルギーは運動量(とスピン)で決まる

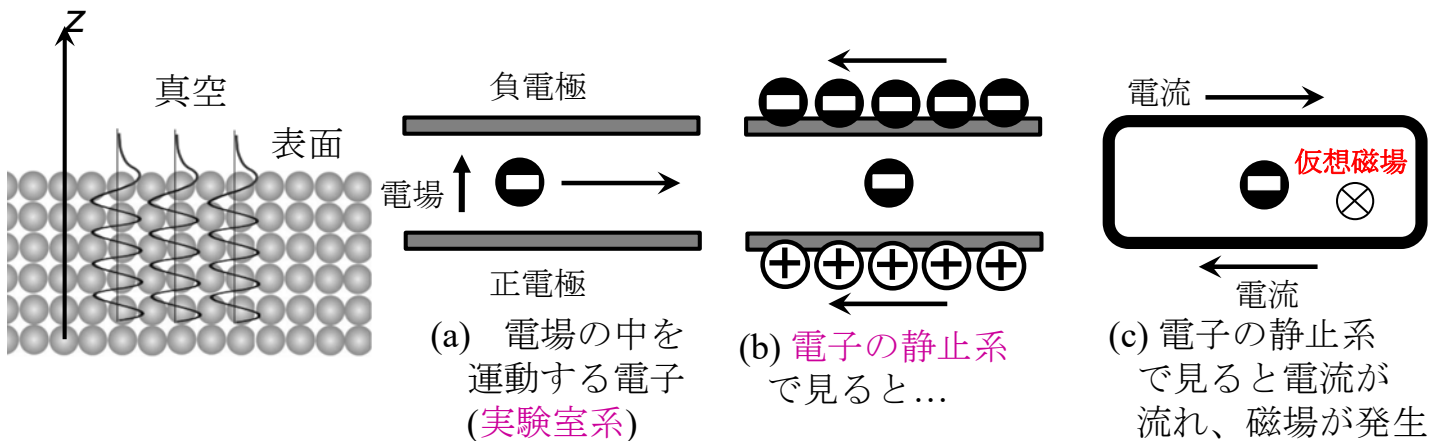


時間反転対称性 + 空間反転対称性 \Rightarrow スピン (Kramers) 縮退

表面電子状態ではスピン分裂 $\leftarrow E(k, \uparrow) \neq E(k, \downarrow)$

表面電子の運動によるスピン軌道相互作用

結晶表面近傍で運動する電子には仮想磁場がかかっている。



$$H = \frac{1}{2m} p^2 + V(x) + \frac{1}{4mc^2} \sigma \cdot (\underbrace{\text{grad } V \times p}_{\text{仮想磁場}})$$

仮想磁場と電子のスピンが相互作用

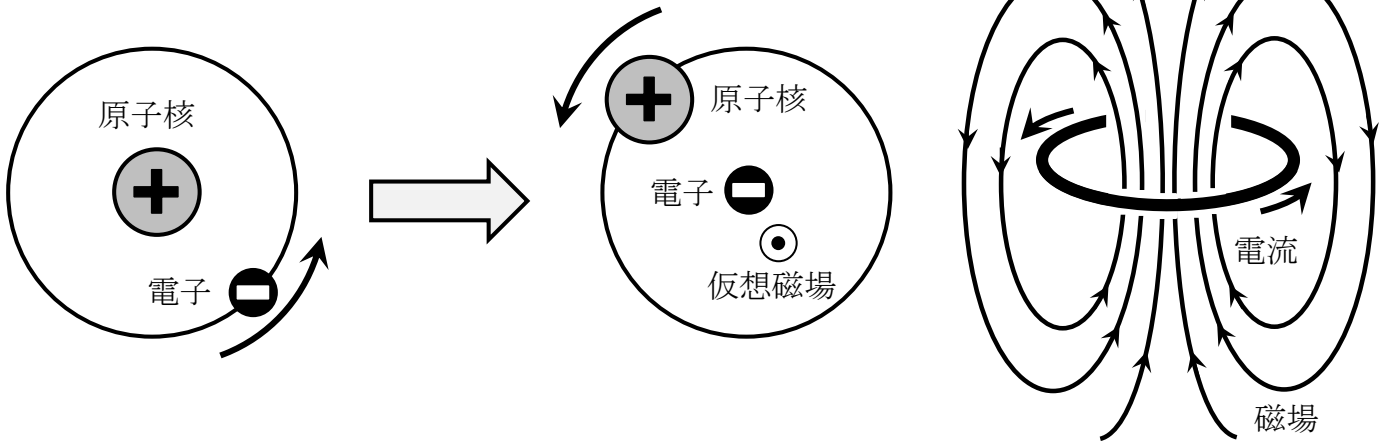
\Rightarrow スピンの向きによってエネルギーが異なる

仮想磁場

\Rightarrow 仮想磁場は表面に平行方向
しかも、電子の運動方向と直交

\Rightarrow スピン運動量 locking
spin \perp momentum

原子軌道でのスピン軌道相互作用



(a) 実験室系

(b) 電子の静止系

(c) 電子が感じる
仮想磁場

$$H = \frac{1}{2m} p^2 + V(x) + \frac{1}{4mc^2} \sigma \cdot (\underbrace{\text{grad } V \times p}_{\text{仮想磁場}})$$

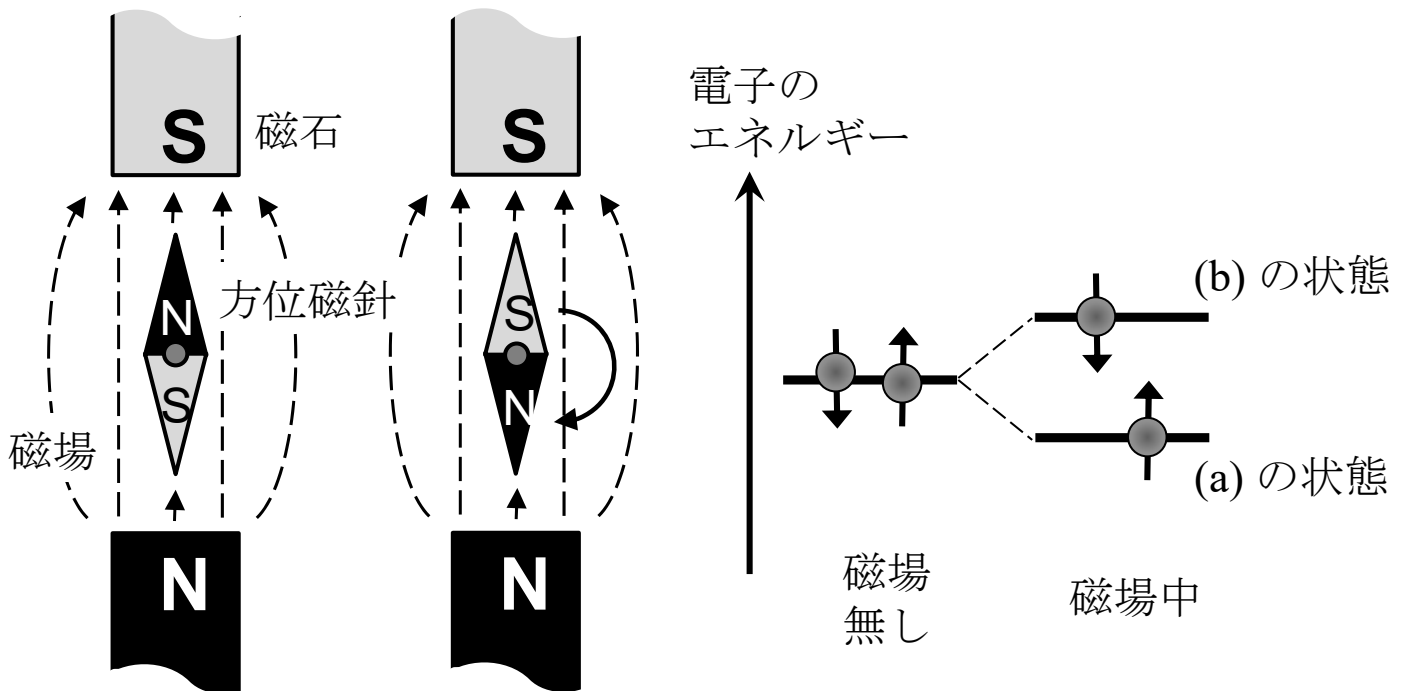
仮想磁場：z 方向
 ⇒ 電子のスピン：z 方向
 電子の運動：xy 面内

仮想磁場と電子のスピンが相互作用
 ⇒ スピンの向きによってエネルギーが異なる

⇒ スピン運動量 locking
 spin ⊥ momentum

Zeeaman 効果 スピンが磁場に平行か反平行かでエネルギーが異なる

← リアルな磁場



Rashba効果/topological絶縁体

スピン軌道相互作用に起因する仮想磁場

⇒ スピンの向きによってエネルギーが異なる

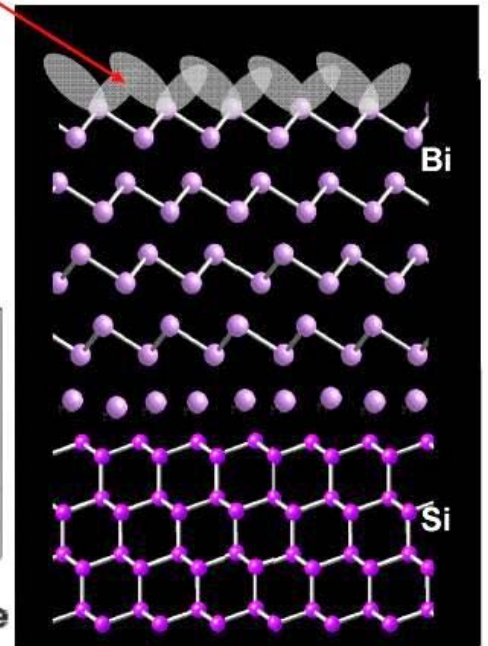
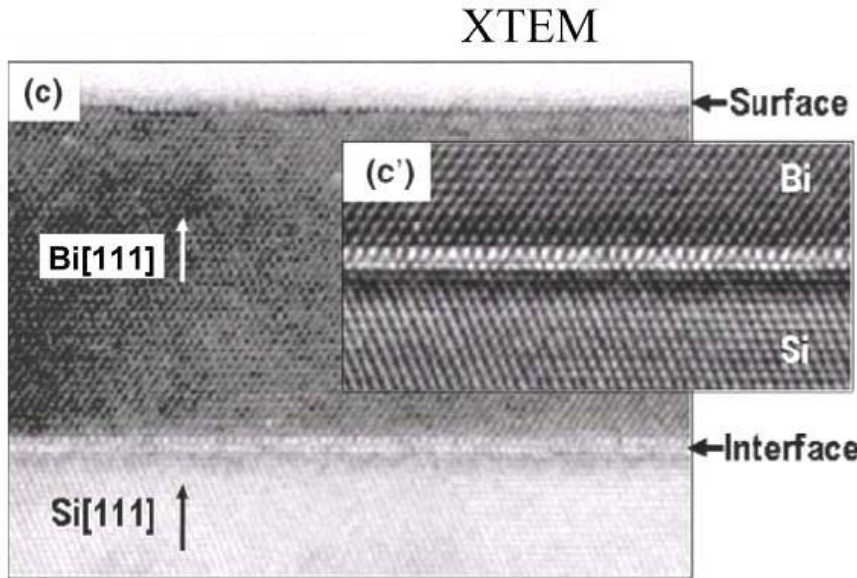
Atomically Flat Ultrathin Bi Film on Si(111)-7 × 7

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

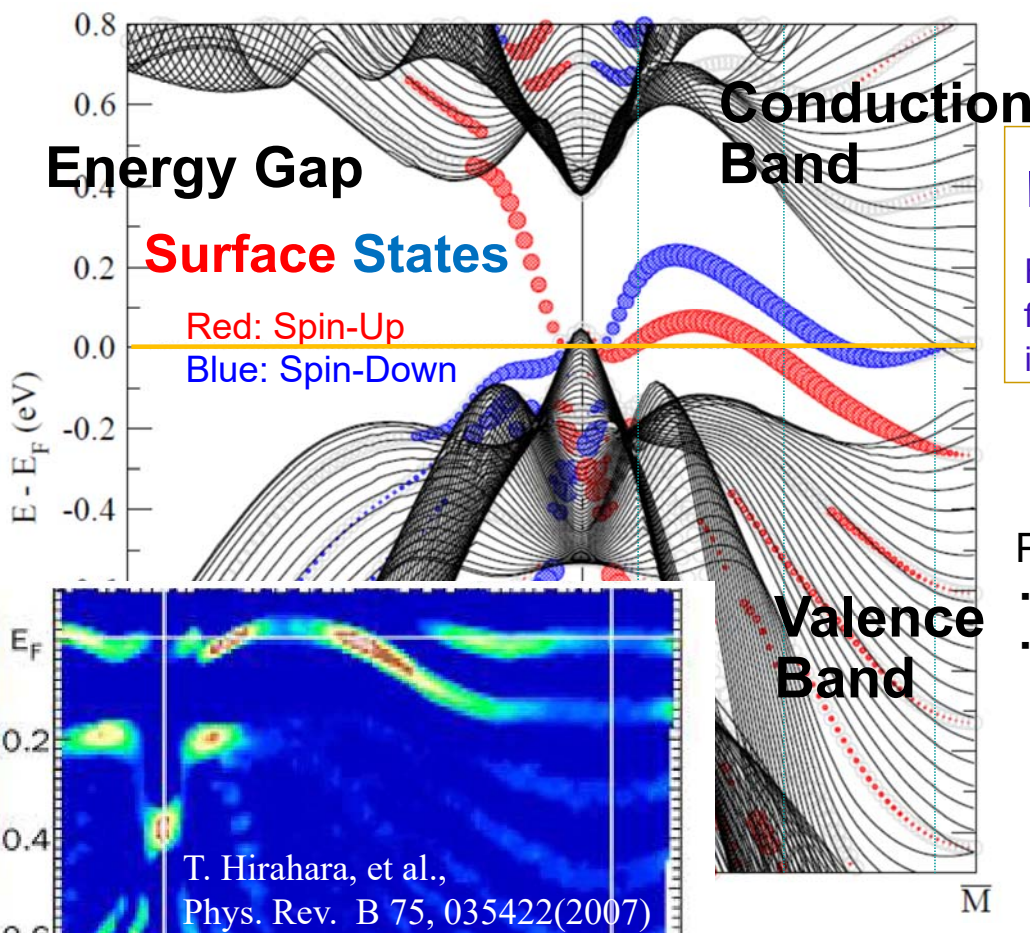
T. Nagao *et al.*,
Surf. Sci. **590**, L247-252 (2005).

- Epitaxial growth of Bi(111) on a wetting layer on Si(111).
- Surface states come from dangling bonds.

Surface States



Bi(111) 20ML-thick Film (1st Principles Cal.)



Dr. G. Bihlmayer
(Julich, Germany)

vacuum
Bi
vacuum
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

T. Hirahara, et al.,
Phys. Rev. B **75**, 035422(2007)

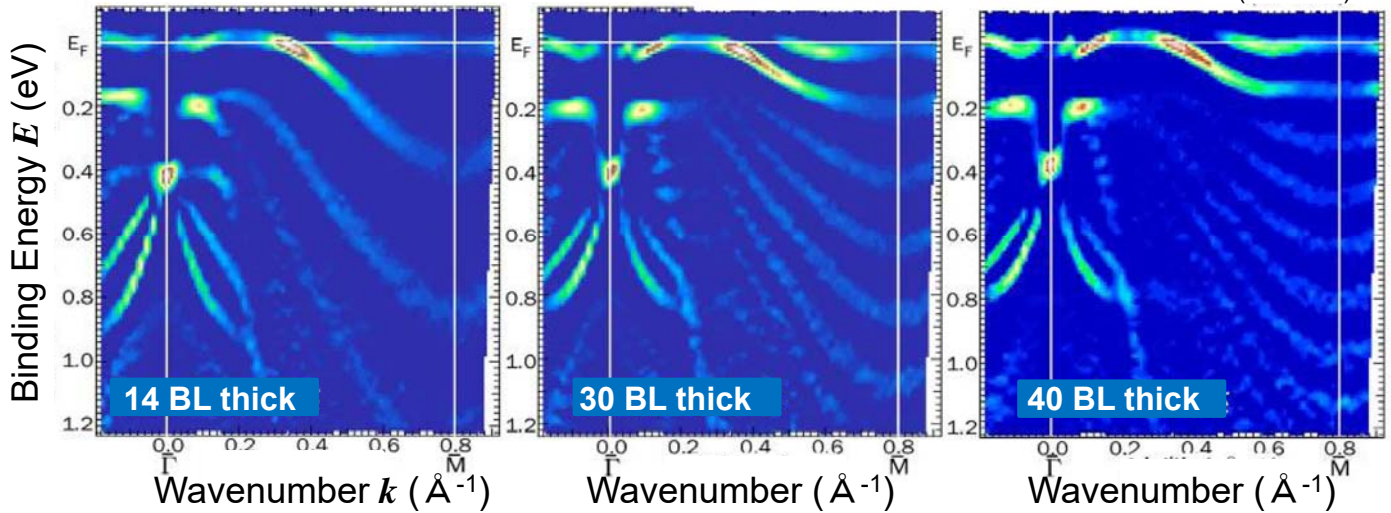
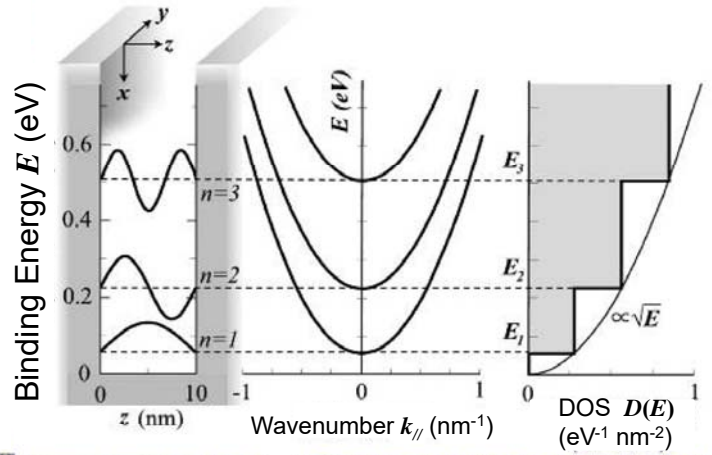
ARPES of Bi(111) Ultrathin films —QWS and SS—

T. Hirahara, et al.,
Phys. Rev. Lett. **97**, 146803 (2006).

Quantum-Well States
Surface States

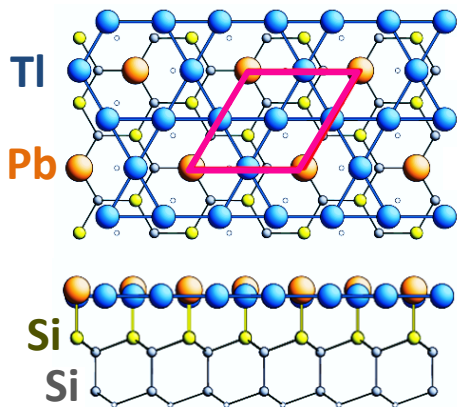


Conductivity of Bi thin film
= surface-state conductivity



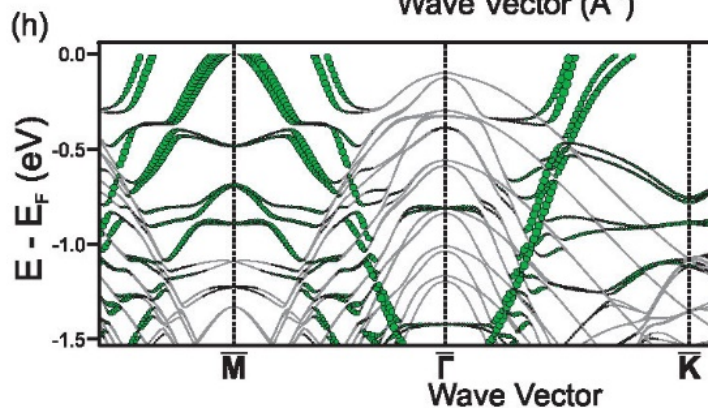
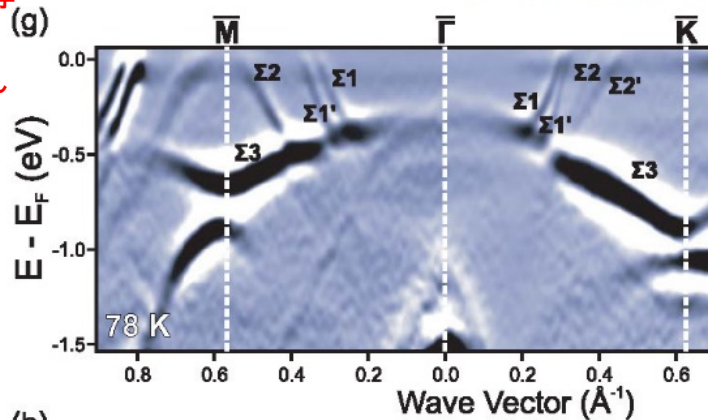
Si(111)-√3x√3-(TI, Pb) 表面構造でのRashba効果と超伝導

A.V. Matetskiy, et al.; PRL **115**, 147003 (2015).

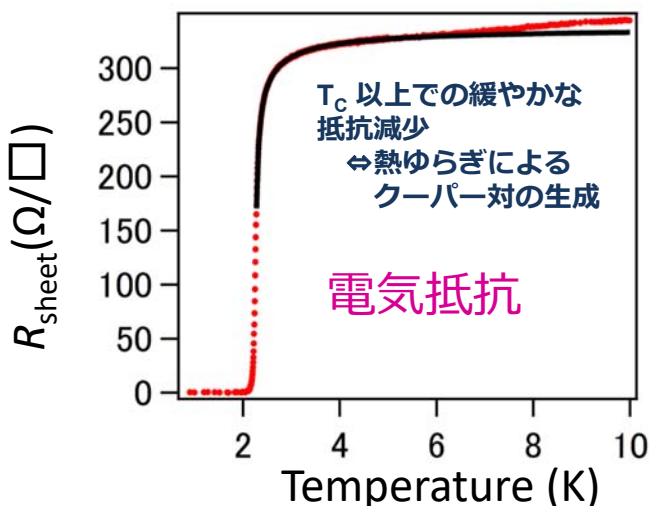


ラシュバ超伝導
→
パリティの破れた超伝導
=
非BCS超伝導
トポロカル超伝導

角度分解光電子分光実験 ARPES

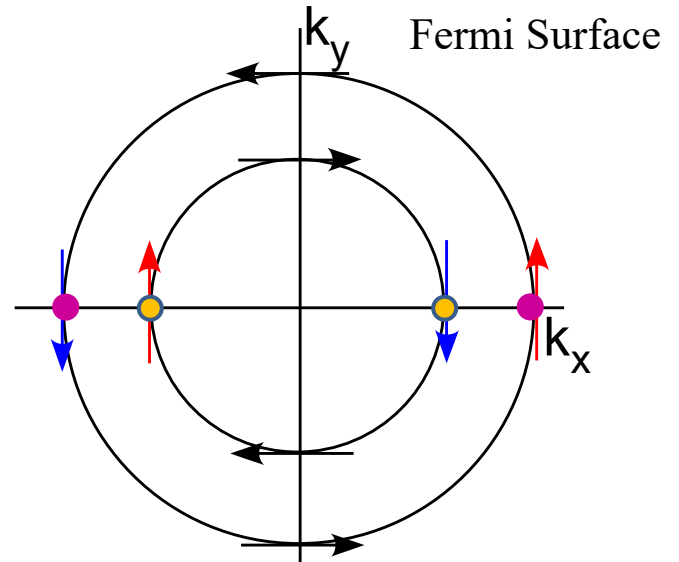
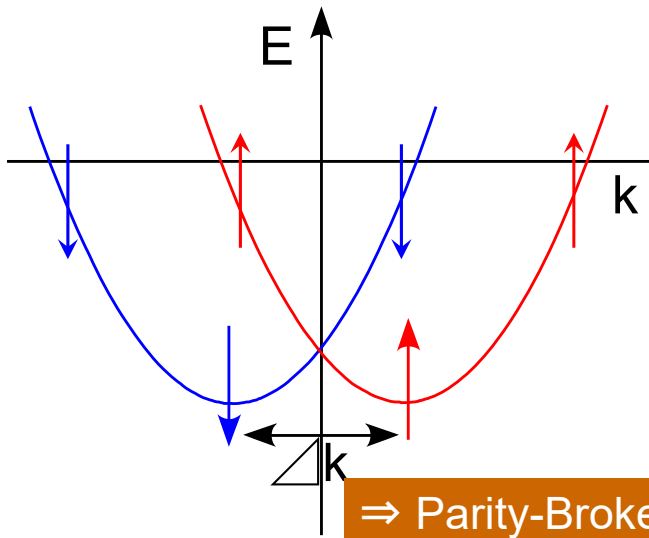


第1原理理論計算



Spin Split and Cooper Pairs in Free-Electron Band

Band Dispersion



⇒ Parity-Broken Superconductors

$$|k \uparrow \rangle | -k \downarrow \rangle = \frac{1}{2} \left(\underbrace{|k \uparrow \rangle | -k \downarrow \rangle - |k \downarrow \rangle | -k \uparrow \rangle}_{\text{Singlet}} \right) + \frac{1}{2} \left(\underbrace{|k \uparrow \rangle | -k \downarrow \rangle + |k \downarrow \rangle | -k \uparrow \rangle}_{\text{Triplet}} \right)$$

トポロジカル表面電子状態

- (1) バンド反転
- (2) パリティ混合
- (3) ヘリカルディラックコーン
- (4) 純スピン

Topological Surface States

$\text{Bi}_{1-x}\text{Sb}_x, \text{Bi}_2\text{Te}_3, \text{Bi}_2\text{Se}_3,$

Analogue of Edge States in Quantum Hall States (2DEG)

⇒ Extension to 3D Materials

⇐ Strong SO Interaction produces effective B.

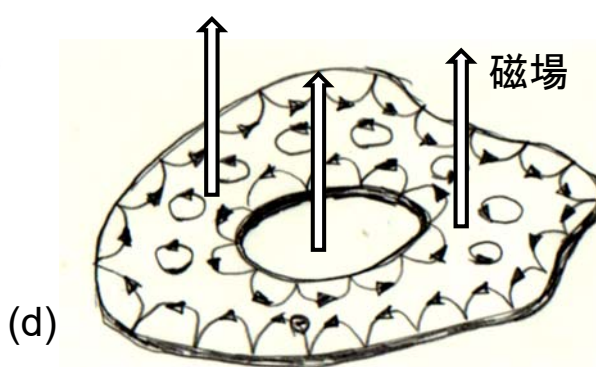
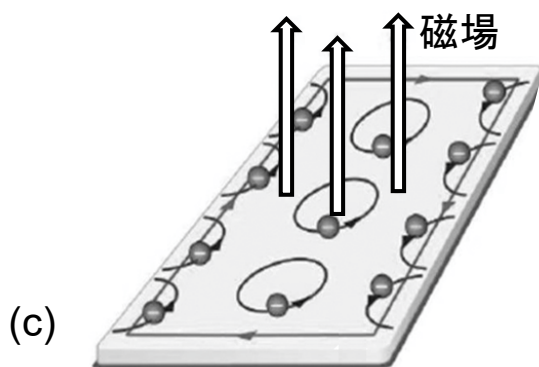
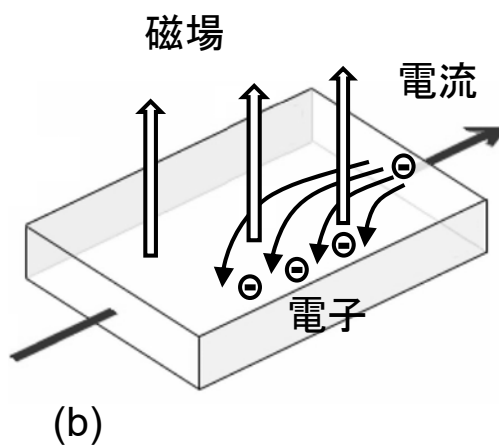
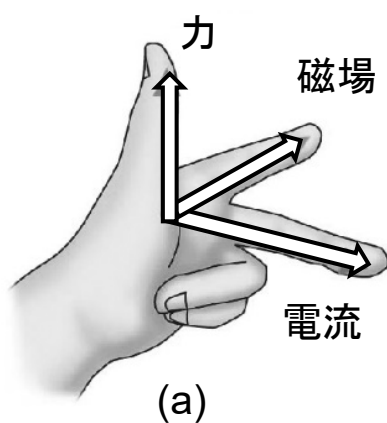
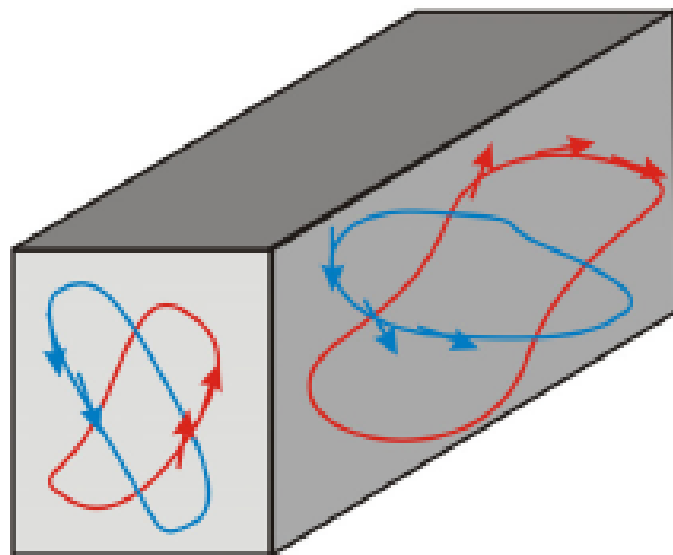
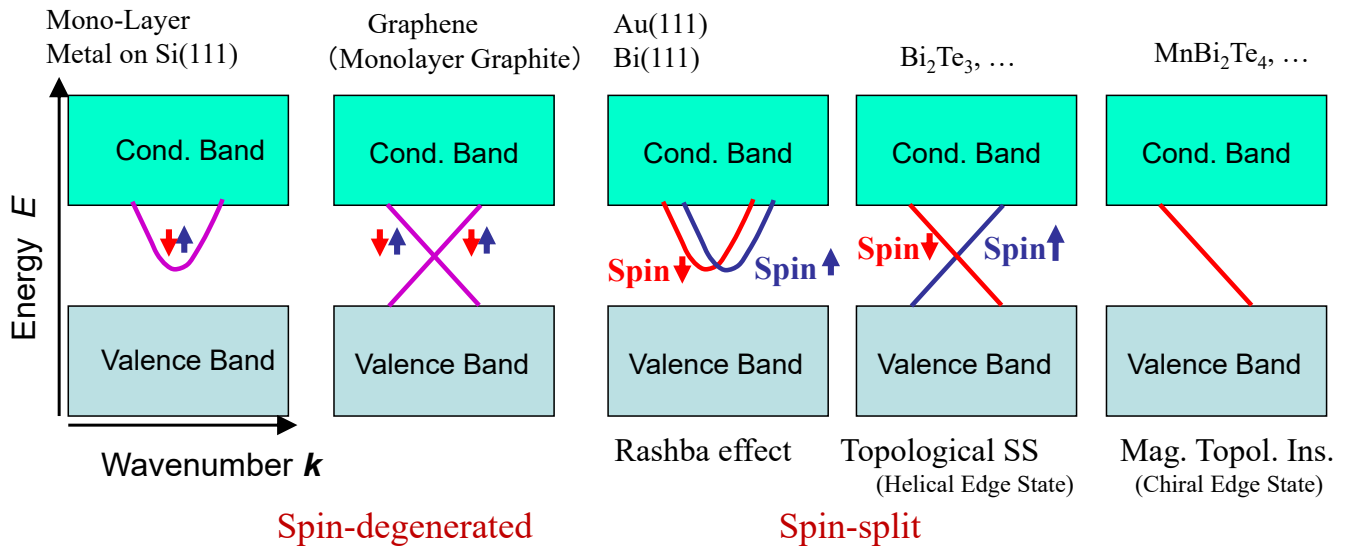


図 1.17. (a) フレミングの左手の法則。磁場のなかを電流が流れるとき、電流が受ける力の方向を示す。(b) ホール効果。磁場によって電子が受ける力で進路が曲げられる。(c) (d) 量子ホール効果の概念図。

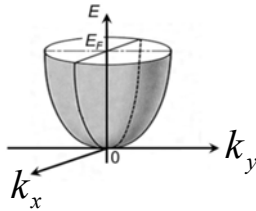
Various Surface States



Free-Electron-like States

(Non-relativistic)

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



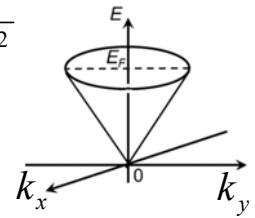
(Relativistic)

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

$$\downarrow m = 0$$

$$E = \pm pc = \pm \hbar ck$$

Massless Dirac Electrons

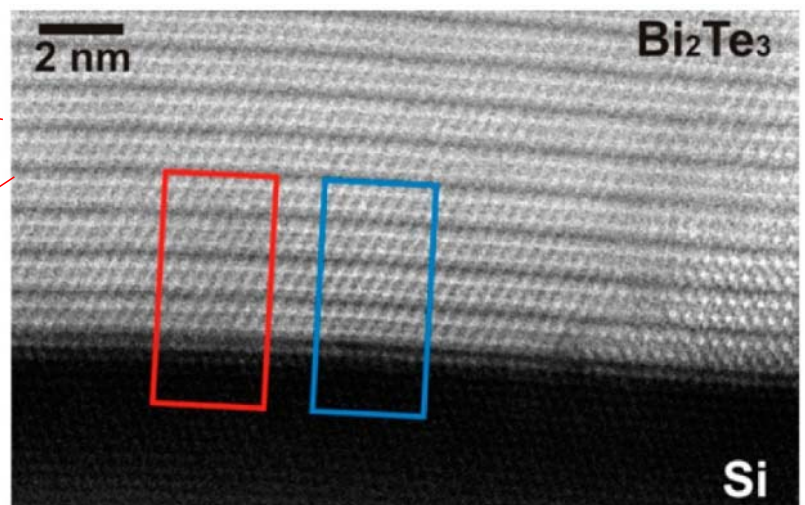
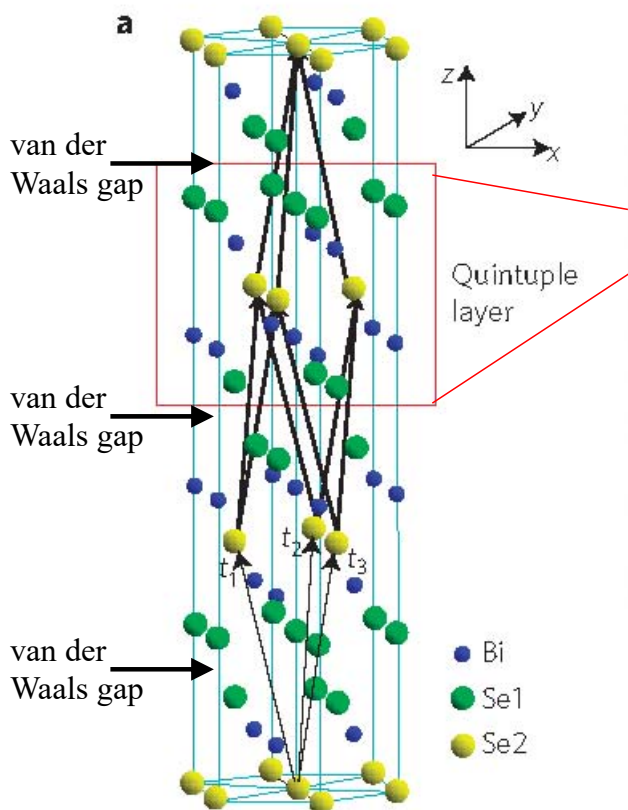


Crystal Structure of Bi₂Se₃ (Bi₂Te₃)

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

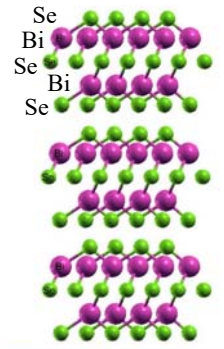
S. Borisova, *et al.*,

Cryt. Growth Des. **12**, 6098 (2012)

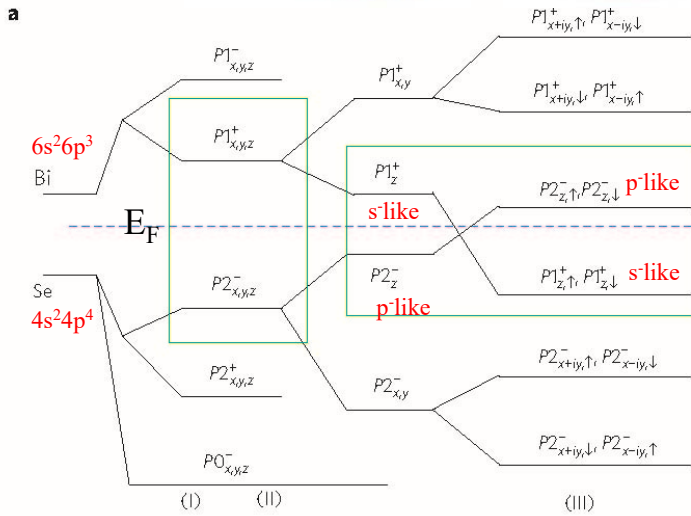


XTEM

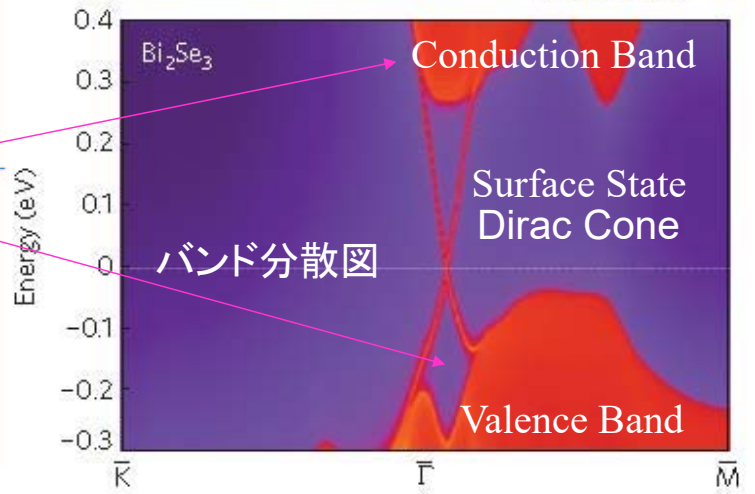
トポロジカル絶縁体: Bi_2Se_3



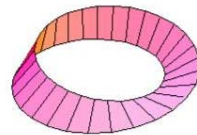
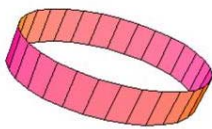
H. Zhang, et al.,
Nature Physics (2009)



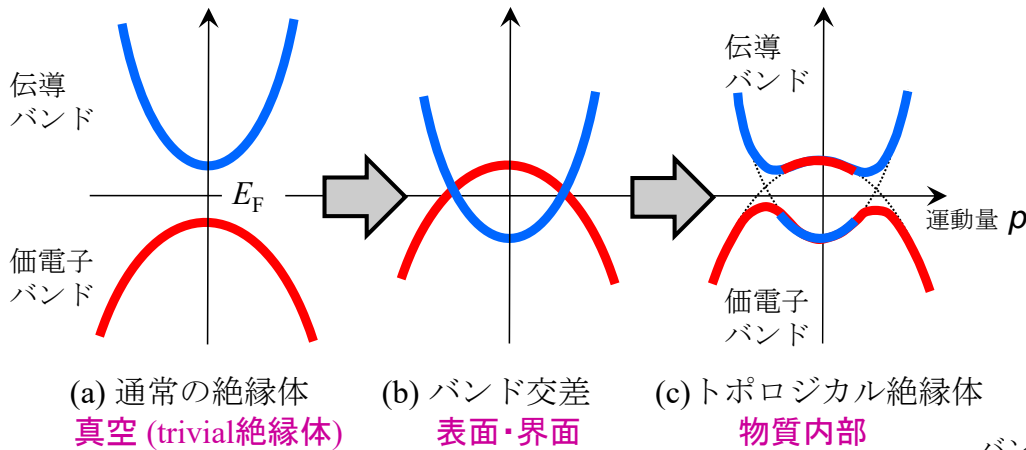
Isolated Atoms (Atomic Orbital) Atomic Bondings Split due to Crystal Field Spin-Orbit Intercation



バンド反転 (強いスピン軌道相互作用)
⇒ パリティが反転.
⇒ トポロジカル物質



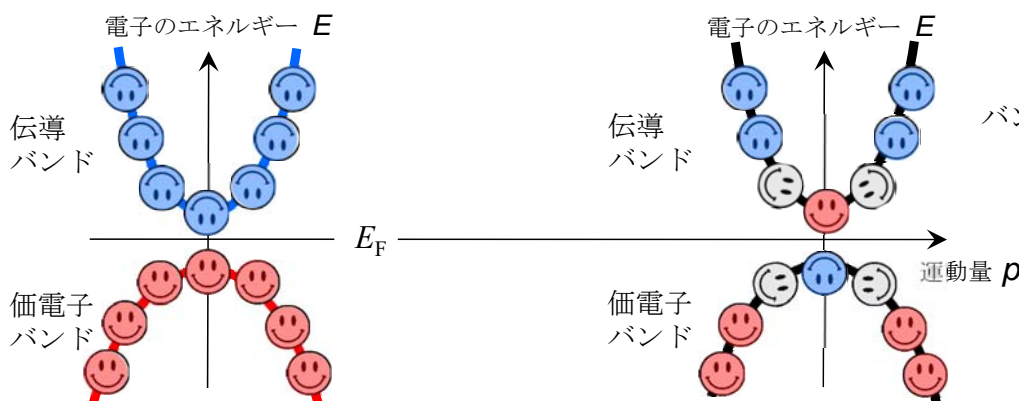
トポロジカル絶縁体と
表面電子状態



(a) 通常の絶縁体
真空 (trivial絶縁体)

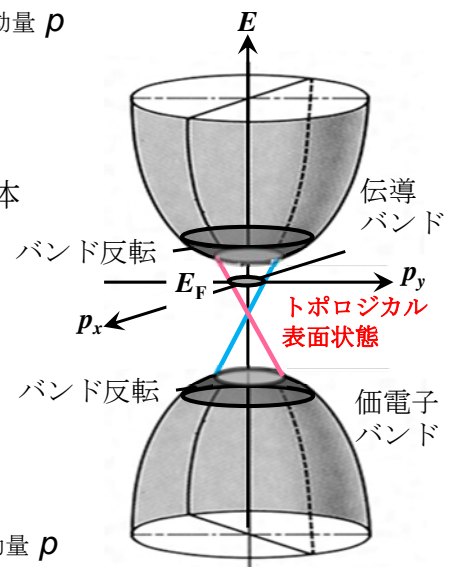
(b) バンド交差
表面・界面

(c) トポロジカル絶縁体
物質内部



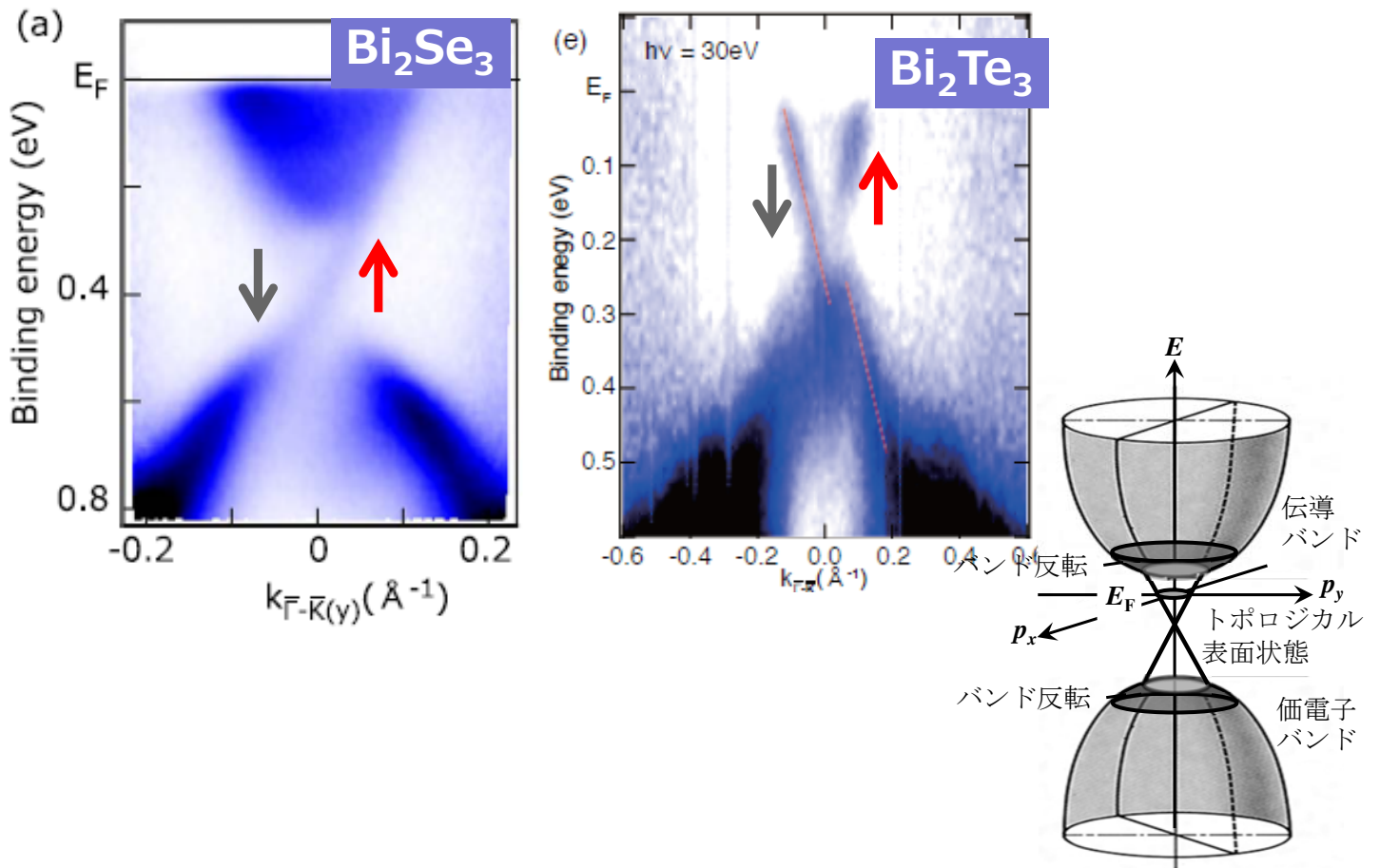
(d) 通常の絶縁体

(e) トポロジカル絶縁体



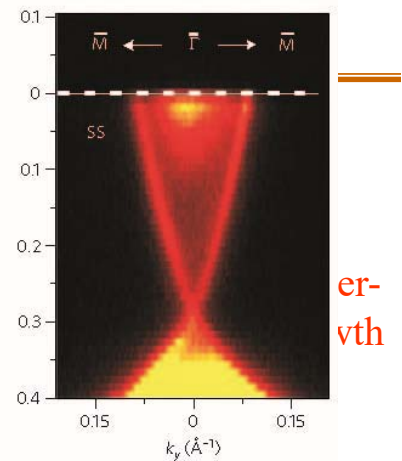
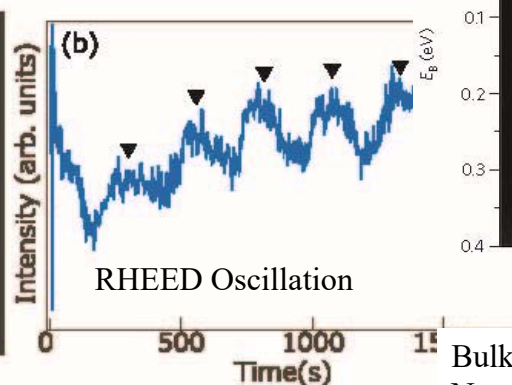
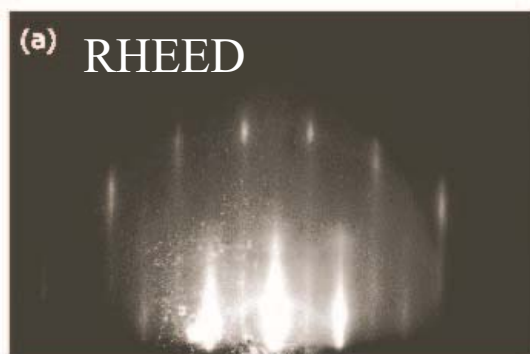
バンドに特異点ができる
→ ベリー曲率 (位相) が生じる

Dirac Cones of Topological Insulators

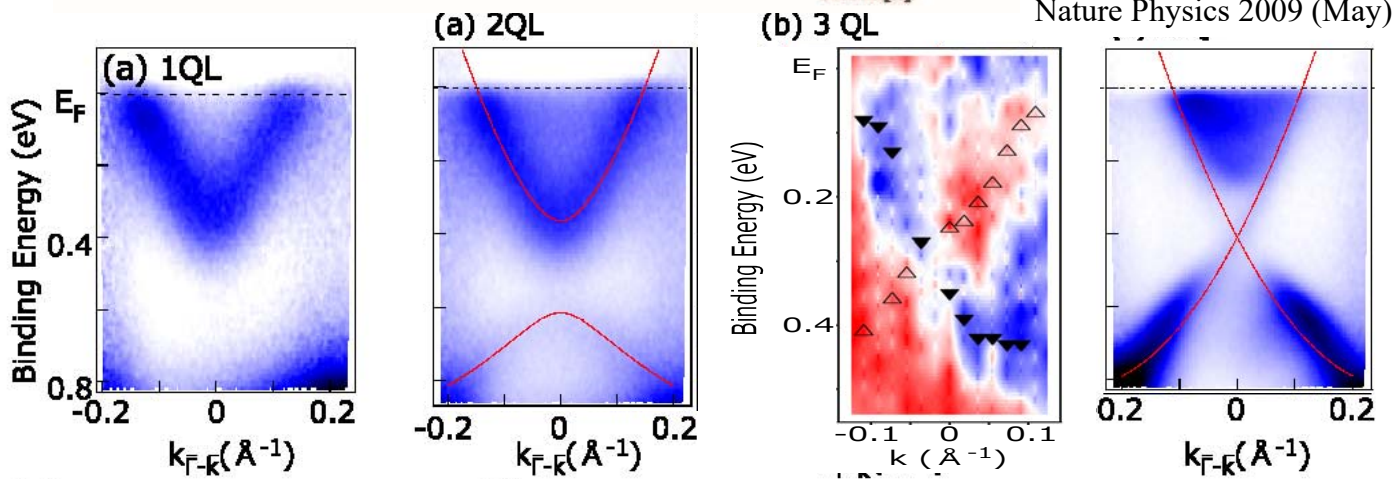


Growth and Band Structure of Bi_2Se_3

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

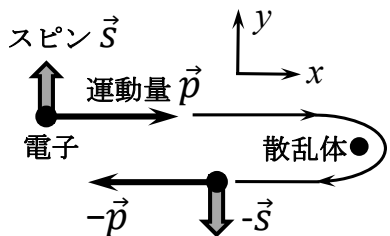


Bulk Crystal Y. Xia, et al., Nature Physics 2009 (May)

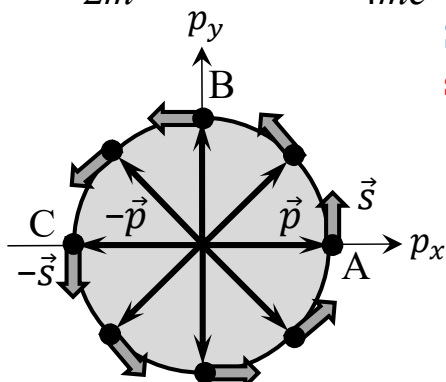


$$H = \frac{1}{2m} p^2 + V(x) + \frac{1}{4mc^2} \sigma \cdot (\text{grad } V \times p)$$

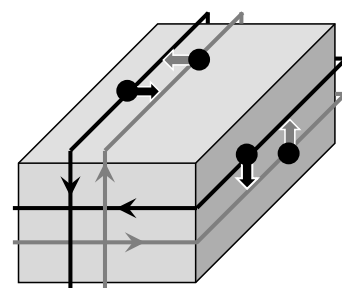
Spin \perp momentum
spin-momentum locking



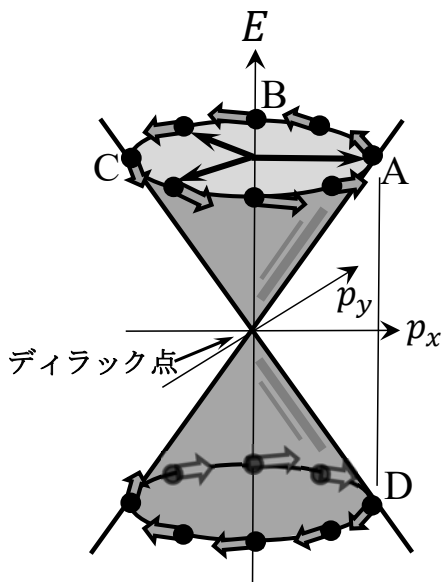
(a) 後方散乱(の禁止)



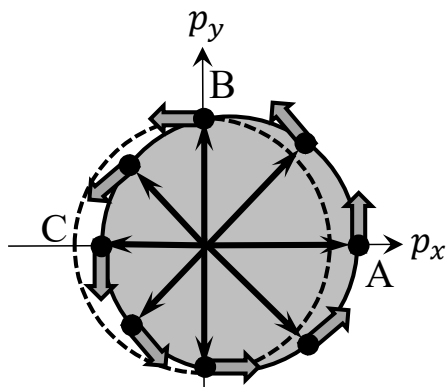
(b) フェルミ面



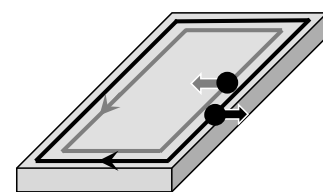
(e) 3D-TI:
表面純スピンの流



(c) ヘリカル Dirac Cone



(d) スピン偏極
電流 (Edelstein効果)

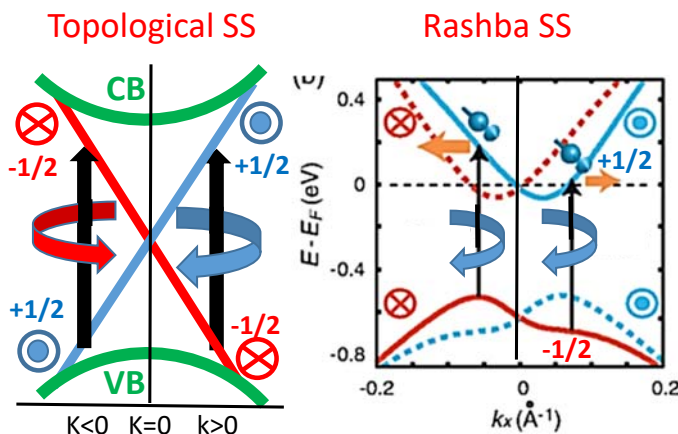
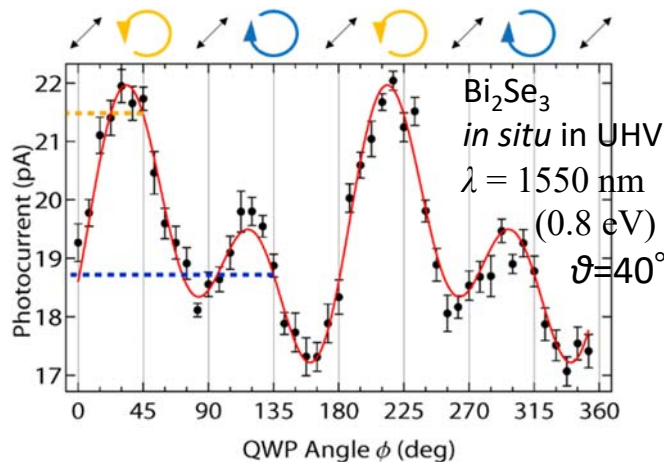
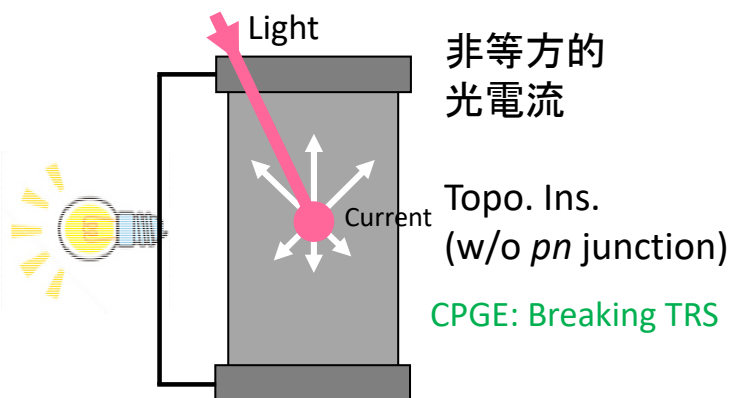
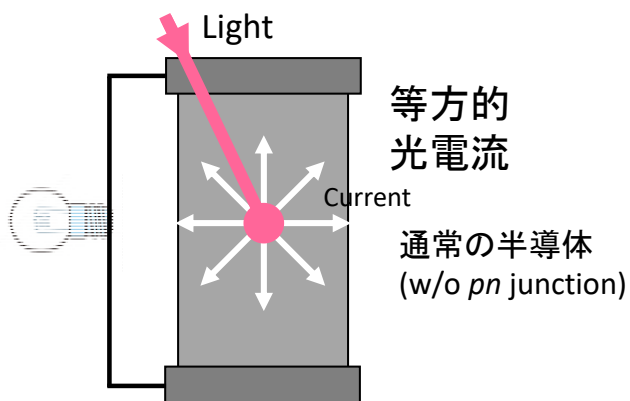


(f) 2D-TI:
エッジ純スピンの流

円偏光照射による非相反光電流

Circular Photo-galvanic Effect (CPGE)

I. Taniuchi, et al., to be published.



電子の位相

(1) ダイナミカル位相

(2) 幾何学的位相 — AB位相

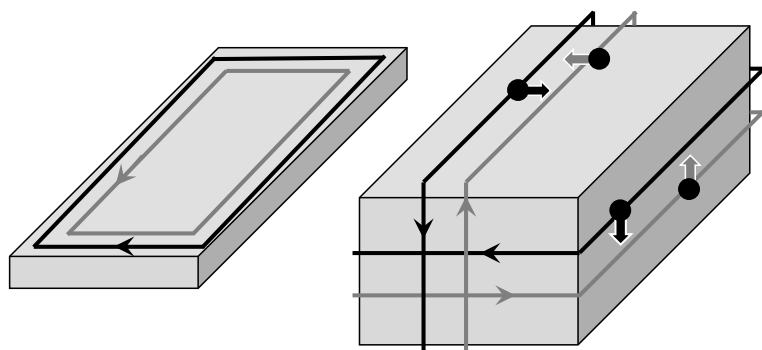
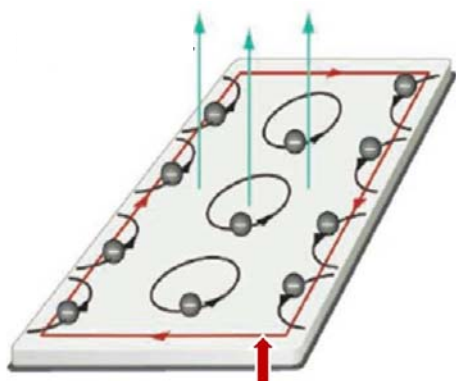
(3) 幾何学的位相 — Berry 位相

電子波の幾何学的位相：AB位相とベリー位相

量子ホール効果

内部は絶縁体(局在)
エッジ・表面は金属

トポロジカル絶縁体



リアル磁場

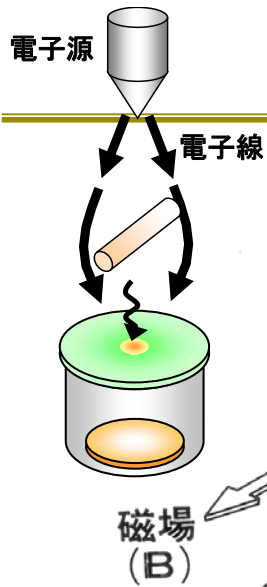
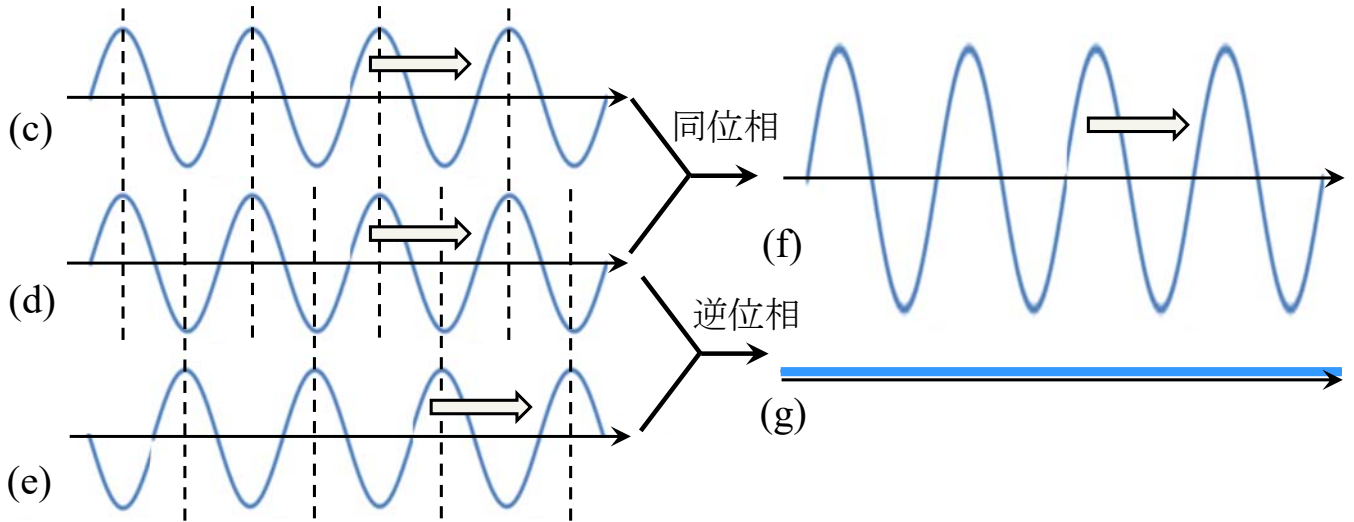
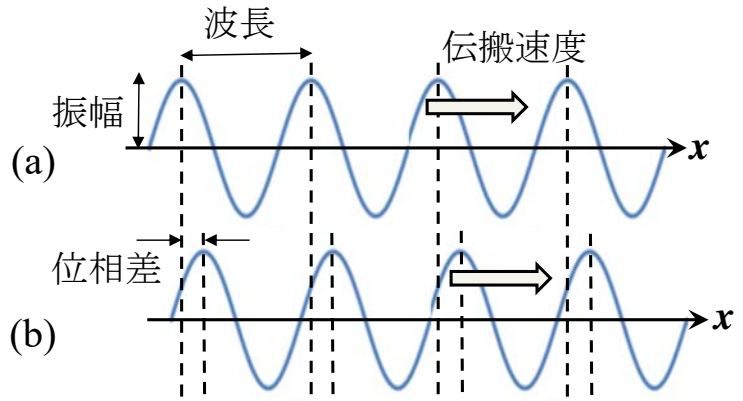
- ⇒ AB位相(幾何学的位相)
- ⇒ 実空間に曲率
- ⇒ トポロジカルに非自明

仮想磁場

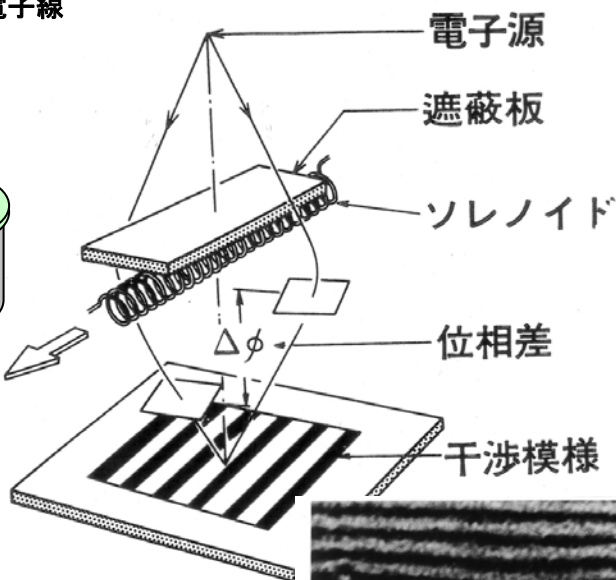
- ⇒ Berry位相(幾何学的位相)
- ⇒ 運動量空間(バンド)に曲率
- ⇒ トポロジカルに非自明

ダイナミカル位相(力学的位相)

波の伝搬に伴って進む位相
 ⇒ 行路の長さの違いによる位相差



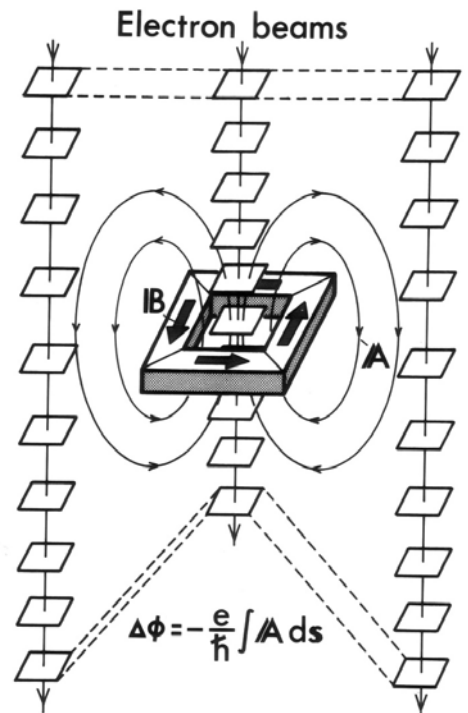
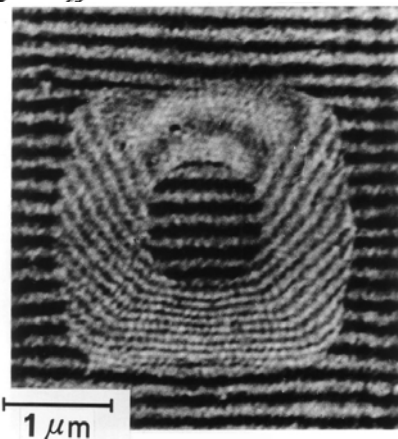
Aharonov-Bohm (AB) 効果の実証実験その1



ベクトル・ポテンシャルによる
 電子波の位相のずれ

$$\Delta\phi = 2\pi \frac{e}{h} \int_{\text{軌道}} \vec{A} \cdot d\vec{r}$$

AB位相



Phase Shift of Electron Beams

外村 彰 (日立), et al
 Physical Review Letters
 48, 1443 (1982)

金属内の伝導電子でのAharonov-Bohm効果

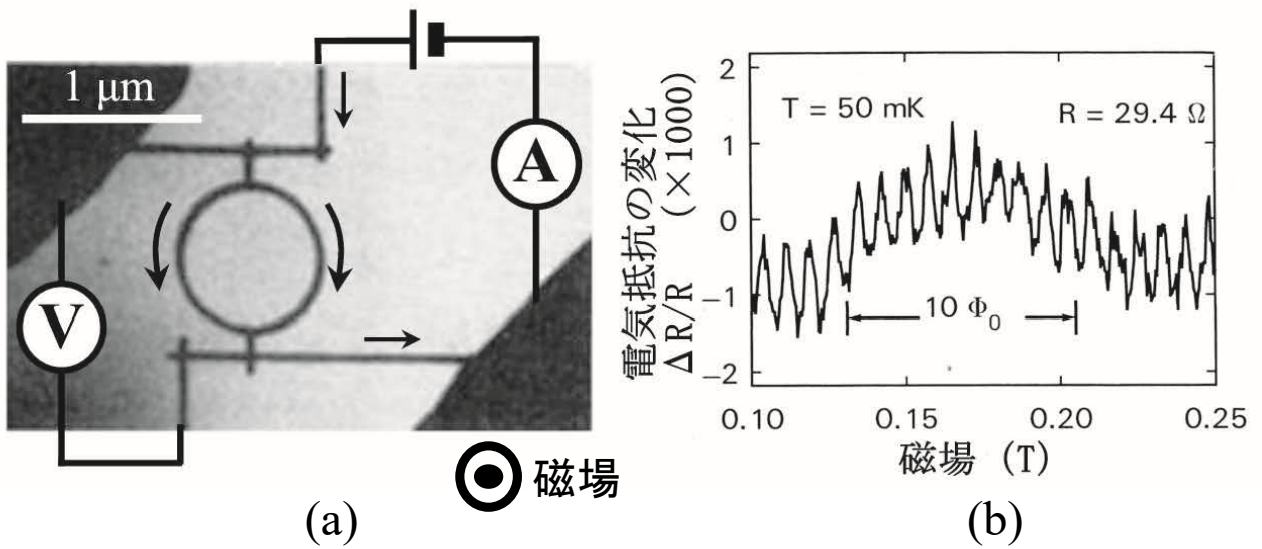
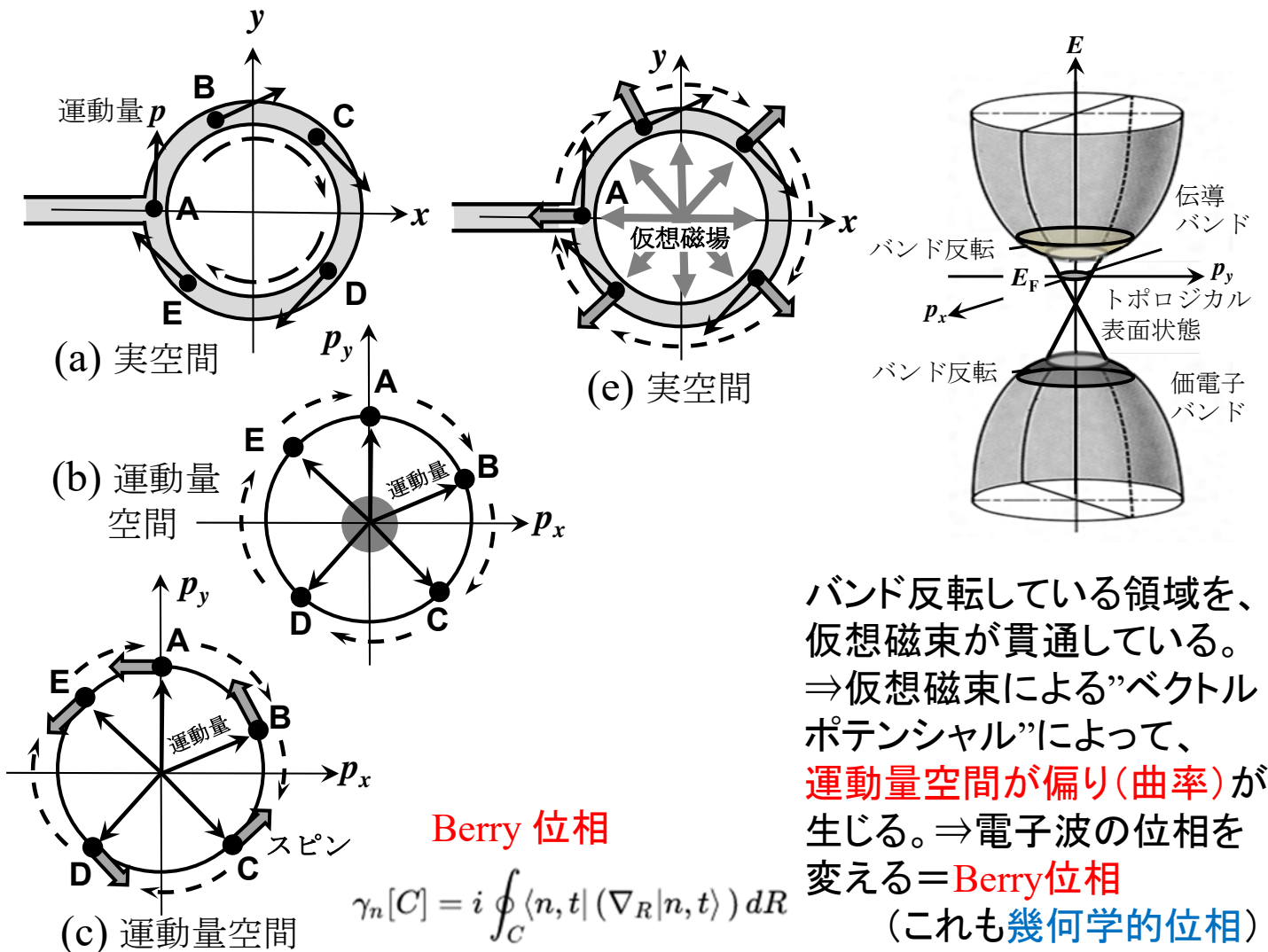


図3.20. アハラノフ=ボーム効果の実験。(a) 測定試料となった金のリング。

(b) 磁場をかけながら測った金の電気抵抗の変化。

(R. A. Webb, et al., Physical Review Letters **54**, 2696 (1985)より転載)。

ベクトルポテンシャルによって空間に偏り(曲率)が生じ、右側のと通路と左側の通路で違いが生じる⇒電子波は、その違いを位相として検出
= AB位相(幾何学的位相)

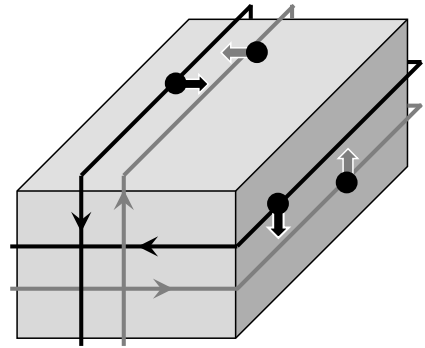
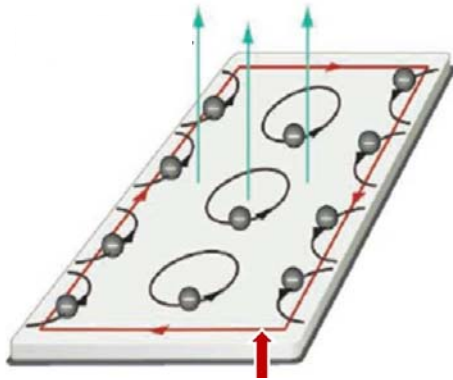


電子波の幾何学的位相：AB位相とベリー位相

量子ホール効果

内部は絶縁体(局在)
エッジ・表面は金属

トポロジカル絶縁体



リアル磁場

- ⇒ AB位相(幾何学的位相)
- ⇒ 実空間に曲率
- ⇒ トポロジカルに非自明

仮想磁場

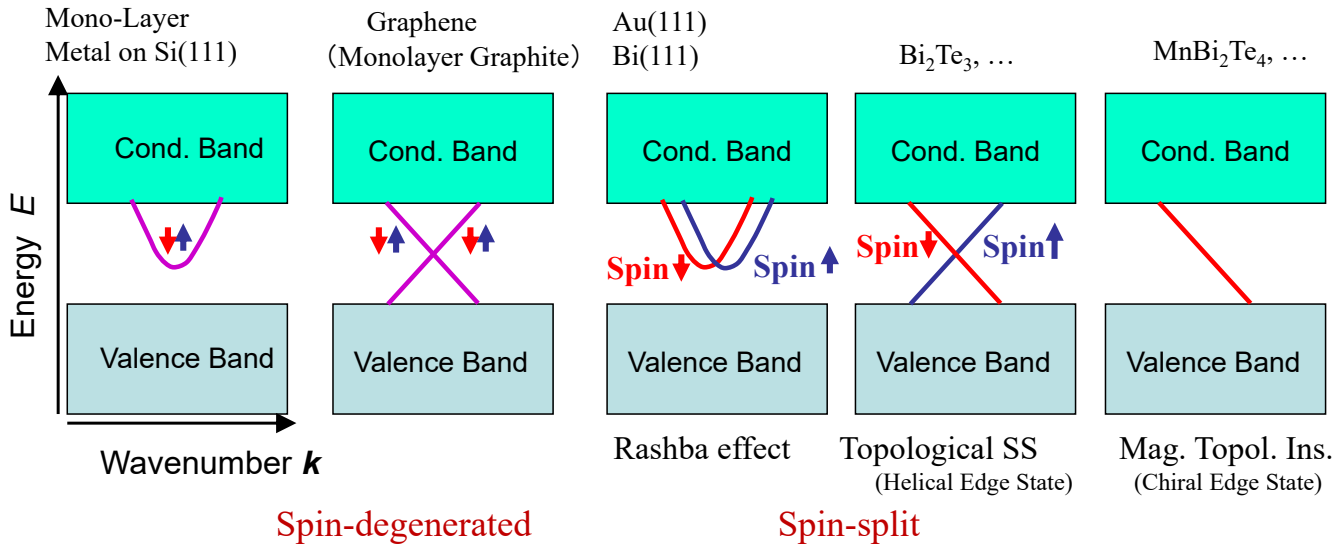
- ⇒ Berry位相(幾何学的位相)
- ⇒ 運動量空間(バンド)に曲率
- ⇒ トポロジカルに非自明

トポロジカル物質ファミリー

(1) 磁性トポロジカル絶縁体

(2) トポロジカル超伝導

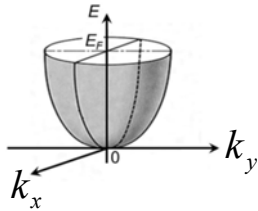
Various Surface States



Free-Electron-like States

(Non-relativistic)

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



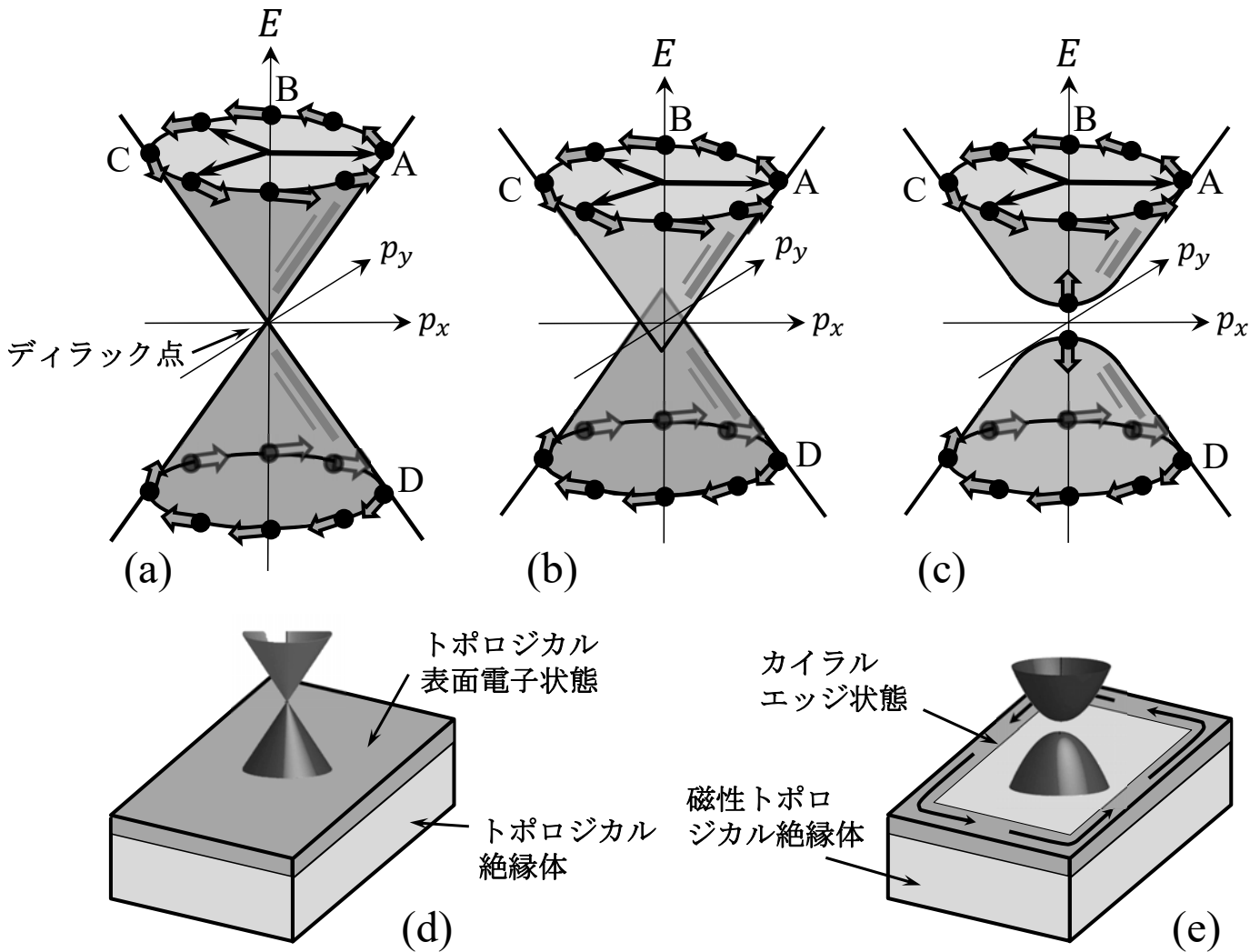
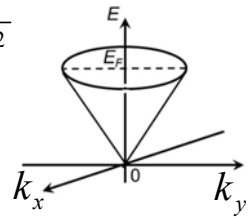
(Relativistic)

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

$$\downarrow m = 0$$

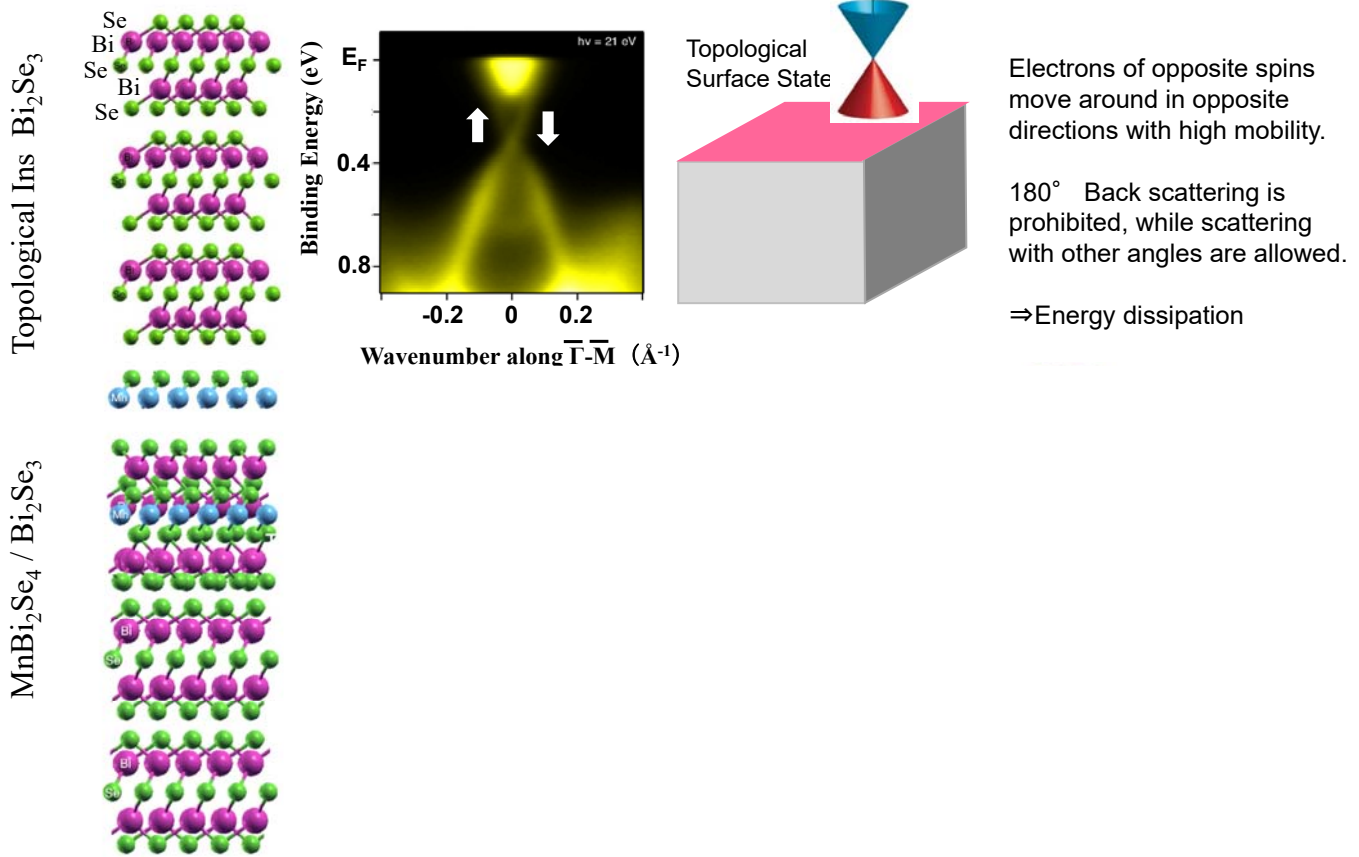
$$E = \pm pc = \pm \hbar ck$$

Massless Dirac Electrons

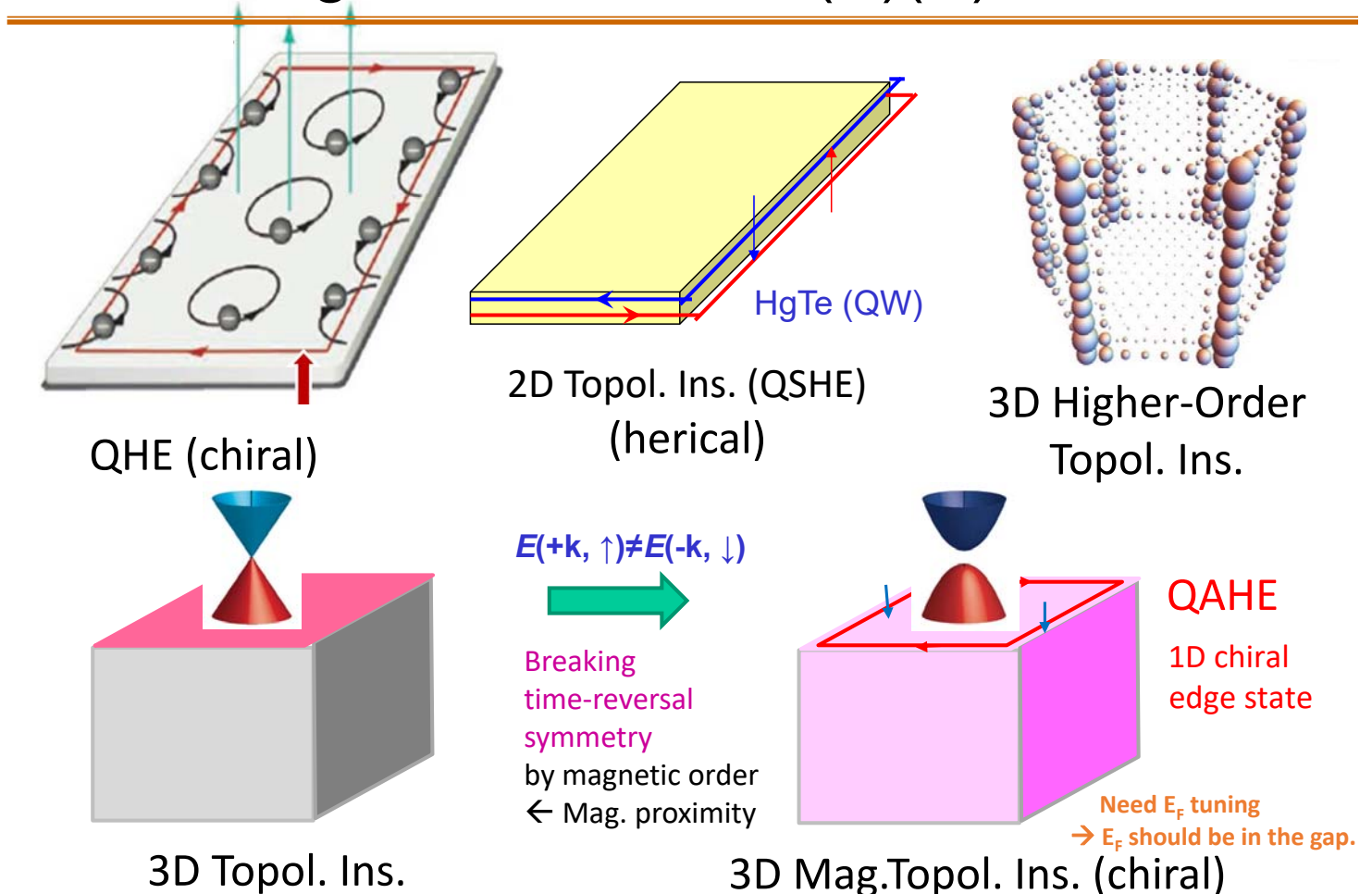


Edge States Toward Quantum Anomalous Hall Eff.

T. Hirahara, et al., Nano Letters 17, 3493 (2017)

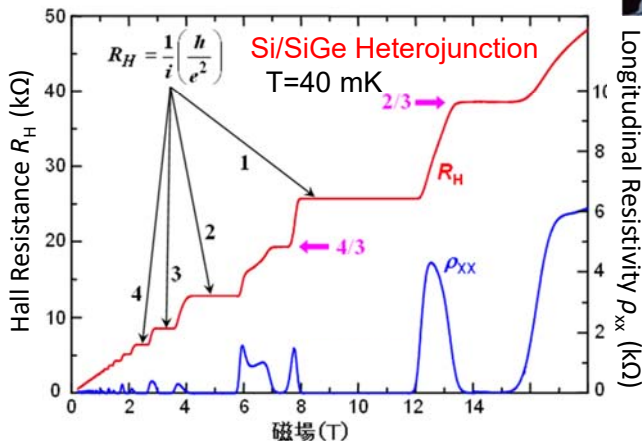
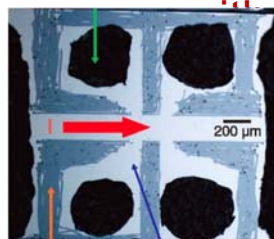
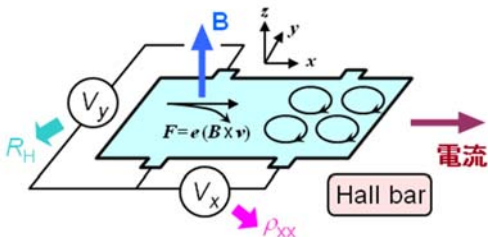


Edge Currents at Q(A)(S)HE



Quantum Hall Effect at 2DEG under strong external mag. field

from Okamoto Lab



- Hall Resistance : quantized in unit of h/e^2
- Longitudinal Resistance : vanishes

Hall Resistance Quantized in unit of h/e^2

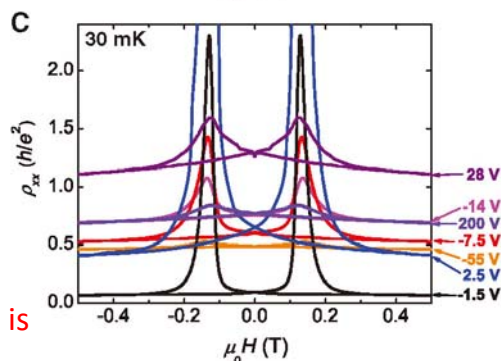
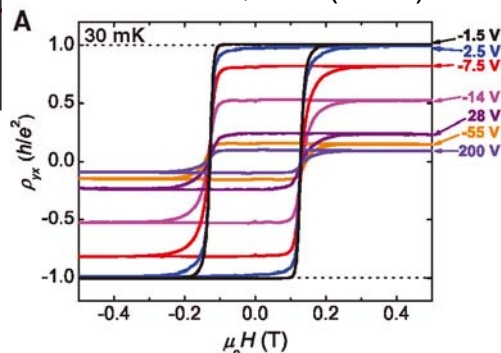
Longitudinal Resistivity Vanishes

Mag. Proximity to break TRS
But, bulk doping is Inhomogeneous.

Magnetic Topological Insulator

Cr or V doped $\text{Bi}_{1-x}\text{Sb}_x\text{Te}$ without external mag. Field

C. Z. Chang et al., Science 340, 167 (2013)



磁性topological 絶縁体表面でのtopological Hall 効果

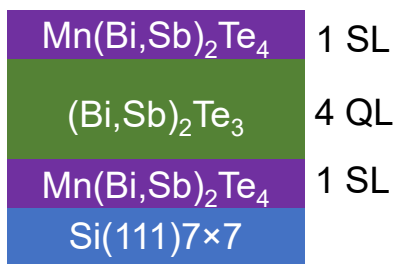
$$\mathcal{H} = \sum_{i,j} J \vec{S}_i \cdot \vec{S}_j + \sum_{i,j} \vec{D} \cdot (\vec{S}_i \times \vec{S}_j)$$

交換相互作用 Dzyaloshinskii-Moriya(DM) 相互作用

T. Takashiro, et al., arXiv 2105.13796

表面界面での空間反転対称性の破れ

分子線エピタキシー法により作製

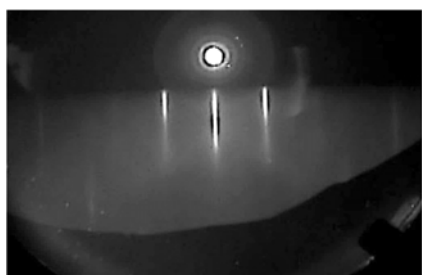
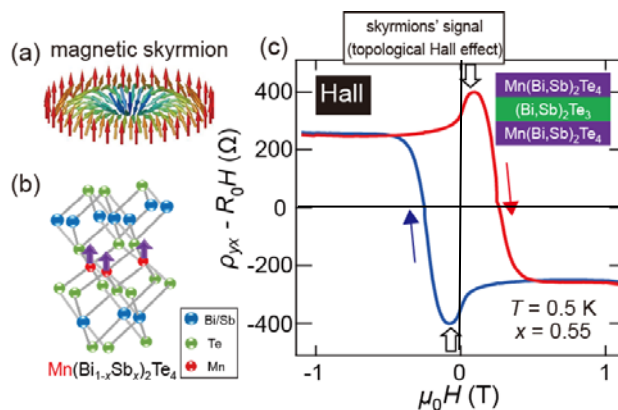


Bi:Sb=0.45:0.55 ⇒ E_F ≈ DP

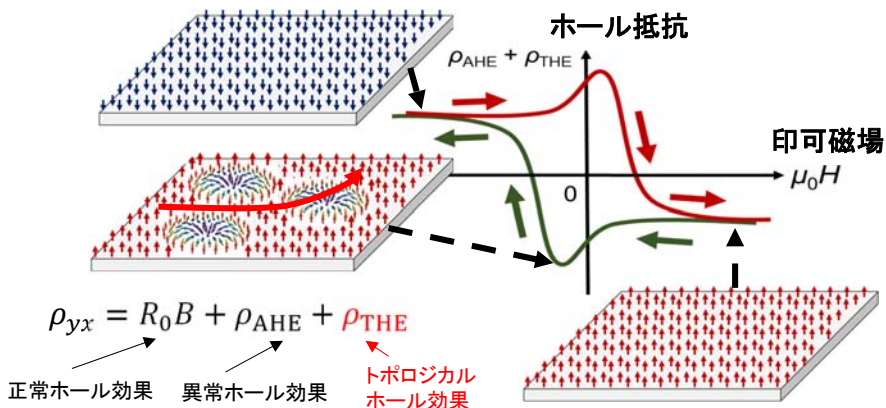
Non-collinear なスピン配置 (skyrmions)

Berry位相

Topological Hall効果



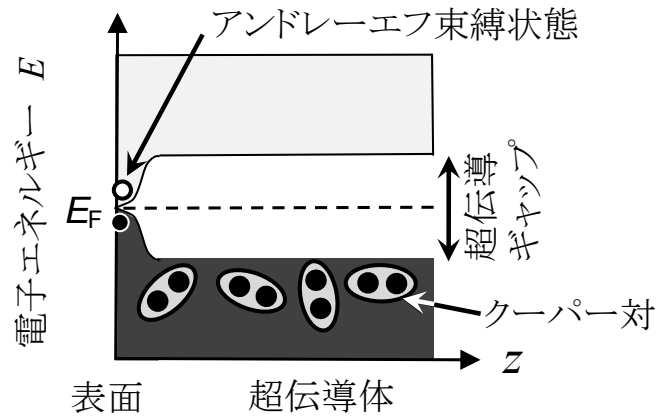
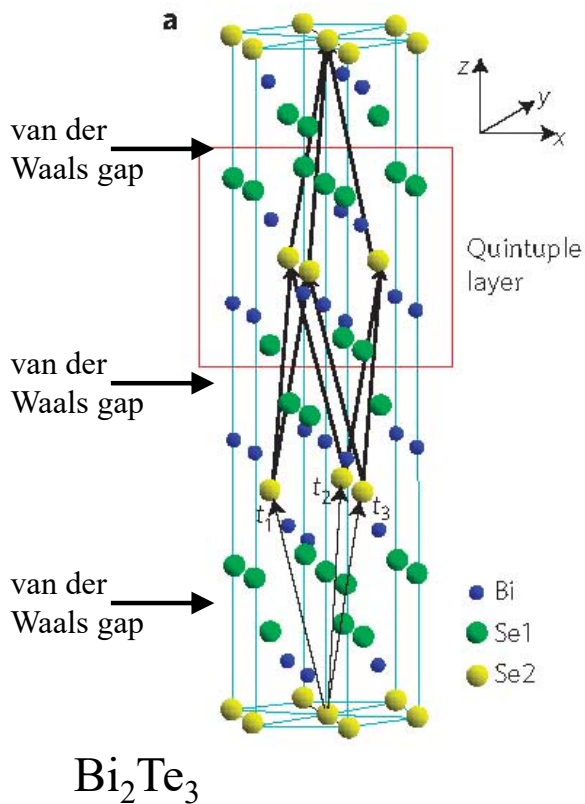
上面Mn(Bi_{0.45}Sb_{0.55})₂Te₄ 成膜後のRHEED pattern



Topological 超伝導

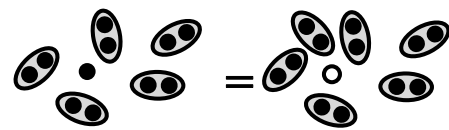
Bi₂Te₃のVan der Waals gapに
Cu 原子をインターカレーション

S. Sasaki, et al., PRL 107, 217001 (2011)



● = ○ + ●

電子 正孔 クーパー対



粒子(電子) = 反粒子(ホール)
Majorana fermion

Summary

— トポロジカル物質：表面物理学の観点から —

トポロジカル表面状態は頑強
スピンの主役

スピン偏極電流

スピンの電流を制御

純スピン流

⇒ スピントロニクス

エッジ伝導 (2次元トポロジカル絶縁体、磁性TI)

無散逸流

