Transport Studies of Epitaxial Thin Films
of Topological Crystalline Insulators

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Outline

- Topological Crystalline Insulator (TCI)
- MBE growth of SnTe on Bi$_2$Te$_3$
- Transport properties of SnTe thin films
Collaborators at Osaka Univ.

Yoichi Ando

Kouji Segawa

Satoshi Sasaki
Z₂ Topological Insulator

vs.

Topological Crystalline Insulator

Two important ingredients for TI:
1) Spin-Orbit Coupling ⇒ band inversion
2) Time Reversal Symmetry ⇒ Kramers’ degeneracy at TRIMs

Two important ingredients for TCI:
1) Spin-Orbit Coupling ⇒ band inversion
2) Symmetry of the crystal lattice ⇒ degeneracy at mirror planes, etc.
SnTe as a topological crystalline insulator (prediction)

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SnTe is predicted to be a topological crystalline insulator with mirror symmetry having robust surface states with an even number of Dirac cones on crystal surfaces such as {001}, {110} or {111}, which are symmetric about {110} mirror planes.

Okada et al., arxiv 1305.2823
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SnTe as a topological crystalline insulator (ARPES)

Tanaka et al.,

Pb$_{0.6}$Sn$_{0.4}$Te
Xu et al.,

Pb$_{0.77}$Sn$_{0.23}$Se
Dziawa et al.,
2D transport in SnTe?

For SnTe concentration of holes is $\sim 10^{20} \div 10^{21} \text{ cm}^{-3}$

→ it should be a problem to probe 2D transport

Nimtz & Schlicht, Narrow-Gap Semiconductors, 1983
Molecular Beam Epitaxy (MBE)

• surface-to-bulk ratio
MBE growth of SnTe (111) thin films on Bi$_2$Te$_3$

(111) plane

- Close lattice match
- Natural continuation for growth of Sn layer on Te-terminated layer
- p-type SnTe on n-type Bi$_2$Te$_3$

cubic

SnTe $a = 6.3$ Å
BaF$_2$ $a = 6.2$ Å (~1.6%)

“hexagonal”

Bi$_2$Te$_3$ $a^* = 4.386$ Å
SnTe $a^* = a/\sqrt{2} = 4.45$ Å (~1.5%)
MBE growth of SnTe (111) thin films on Bi$_2$Te$_3$

- 2D growth mode
MBE growth of SnTe (111) thin films on Bi$_2$Te$_3$

High structural quality of grown films
2D transport in SnTe thin films grown on Bi$_2$Te$_3$

- No sign of the cubic-to-rhombohedral phase transition
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- 2D character of quantum oscillations
2D transport in SnTe thin films grown on Bi$_2$Te$_3$

\[ k_F = 1.9 \times 10^6 \text{ cm}^{-1}, \quad n_s = 3 \times 10^{11} \text{ cm}^{-2} \]
for each FS (each spin)
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Origin of surface Dirac electrons

- both SnTe and Bi$_2$Te$_3$ have topological SS
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  - heterostructure (common anion rule)
Band lineups in heterostructures

The Nobel Prize in Physics 2000

Zhores I. Alferov
Herbert Kroemer

The n-N Heterojunction

straddling  staggered  broken-gap

$\Delta E_C$  $V_{bi}$  $\varphi_1 - \varphi_2$

$\varphi = \text{work function}$
$\chi = \text{electron affinity}$
$E_G = \text{band gap}$
$E_C = \text{conduction band}$
$E_V = \text{valence band}$
$E_F = \text{fermi level}$
$V_{bi} = \text{built in voltage}$
Origin of surface Dirac electrons

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- $p^+ - n^+$ tunneling junction

![Graph of energy levels and materials](Image)
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- SS is most likely on the free surface of SnTe
SS on the (111) plane of SnTe

Surface States of Topological Crystalline Insulators in IV-VI Semiconductors

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$v_F = 5.6 \times 10^7$ cm/s \quad <v_F> = 2.5 \times 10^7$ cm/s

$1.4 \times 10^7 \quad 4.5 \times 10^7$
SS on the (111) plane of Pb$_{0.6}$Sn$_{0.4}$Te

The topological-crystalline-insulator (Pb,Sn)Te - surface states and their spin-polarization

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(Dated: March 27, 2013)

$v_F = 7 \times 10^7$ cm/s

$\langle v_F \rangle = 3.1 \times 10^7$ cm/s

2.5$\times$10$^7$ 5$\times$10$^7$

Sn-terminated

Te-terminated

ArXiv 1303.7119
Surface termination

- polar catastrophe in SnTe films grown along the (111) direction
Surface termination (Te)

- polar catastrophe in SnTe films grown along the (111) direction
- partially compensated charge on the surfaces

Te-terminated Bi$_2$Te$_3$ surface
Surface termination (Te)

- polar catastrophe in SnTe films grown along the (111) direction
- partially compensated charge on the surfaces
- natural compensation at the interface (p-n junction)
Surface termination (Te)

- polar catastrophe in SnTe films grown along the (111) direction
- partially compensated charge on the surfaces
- natural compensation at the interface (p-n junction)
- upward band bending for Te-terminated surface
Surface termination (Te)

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- natural compensation at the interface (p-n junction)
- upward band bending for Te-terminated surface
- finite electrostatic potential for Te-terminated surface
Surface termination (Sn)

- polar catastrophe in SnTe films grown along the (111) direction
- partially compensated charge on the surfaces
- natural compensation at the interface (p-n junction)
- zero electrostatic potential for Sn-terminated surface
- downward band bending for Sn-terminated surface
Origin of surface Dirac electrons

- Sn-terminated surface
- Downward band bending
- Fermi level crosses Dirac cones at ~0 (Γ) and ~40 meV (M)
- Single frequency $F = 12.3$ T of SdH oscillations
- $v_F = 3.2 \times 10^7$ cm/s (SdH)
Nonlinear Hall effect

- Two-band fitting
- $n_s = 3 \times 3 \times 10^{11} \text{ cm}^{-2}$ (from SdH oscillations) is fixed
- $p_{3D} = 6.4 \times 10^{20} \text{ cm}^{-3}$ (from 300K Hall meas.) is fixed
- High mobility of surface Dirac electrons
• High quality epitaxial SnTe films have been grown on Bi$_2$Te$_3$ buffer layer.

• n- and p-type carriers are found to coexist in SnTe film, which is electrically decoupled from Bi$_2$Te$_3$ layer due to a p-n junction at the interface.

• SdH oscillations combined with the Hall resistivity data provide evidence that the n-type carriers are Dirac fermions residing on the top SnTe (111) surface.