National Institute of Advanced Industrial Science and Technology AIST

技術を社会へ－Integration for Innovation

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Topological heterostructures of layered telluride compounds

Yuta Saito, Kotaro Makino, Paul Fons, Alexander V. Kolobov, and Junji Tominaga

National Institute of Advanced Industrial Science and Technology (AIST)
yuta-saito@aist.go.jp
Department of Engineering, University of Cambridge
ys478@cam.ac.uk

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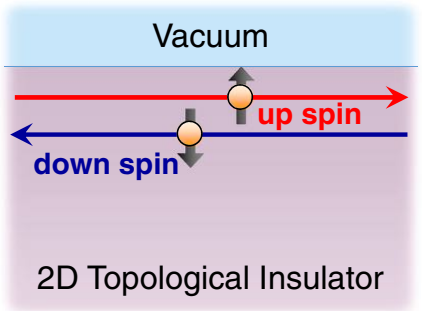
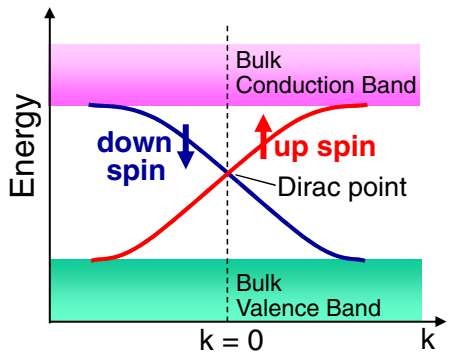
UNIVERSITY OF CAMBRIDGE

Topological insulator (TI)

New matter arisen from topological insulating nature

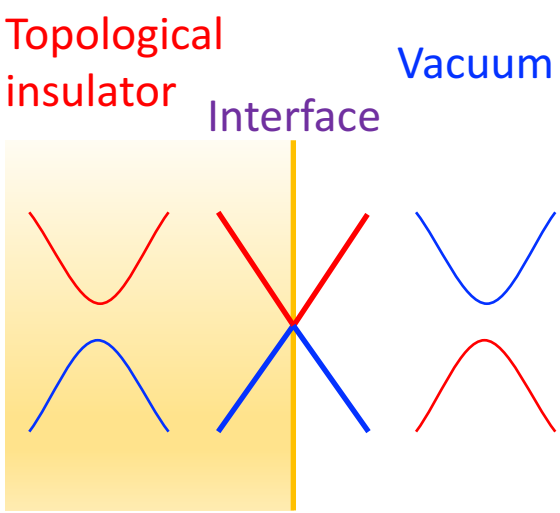




Topological insulator materials

CdTe/HgTe/CdTe (2D), $Bi_{1-x}Sb_x$, Bi_2Se_3, Bi_2Te_3, Sb_2Te_3, $Ge_1Bi_{4-x}Sb_xTe_7$, Bi_2Te_2Se, $TlBiSe_2$, SnTe etc.

Y. Ando, *J. Phys. Soc. Jpn.* **82** (2013) 102001



Strong spin-orbit coupling

⇩

Band inversion in bulk

⇩

The band must cross at the interface resulting in the formation of Dirac cone.

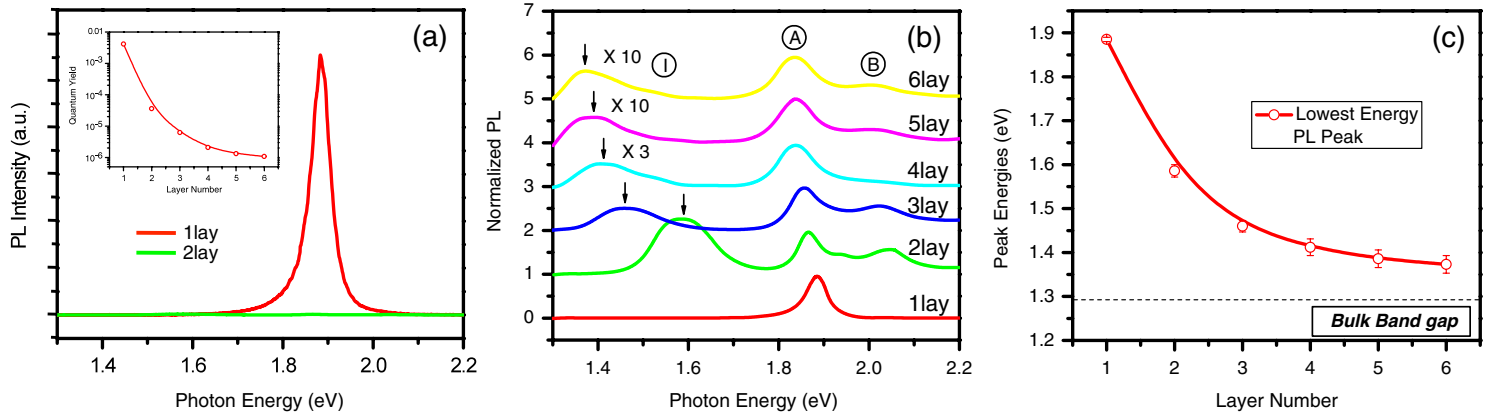
Features
- Dirac cone at the surface
- Helical spin states

⇩

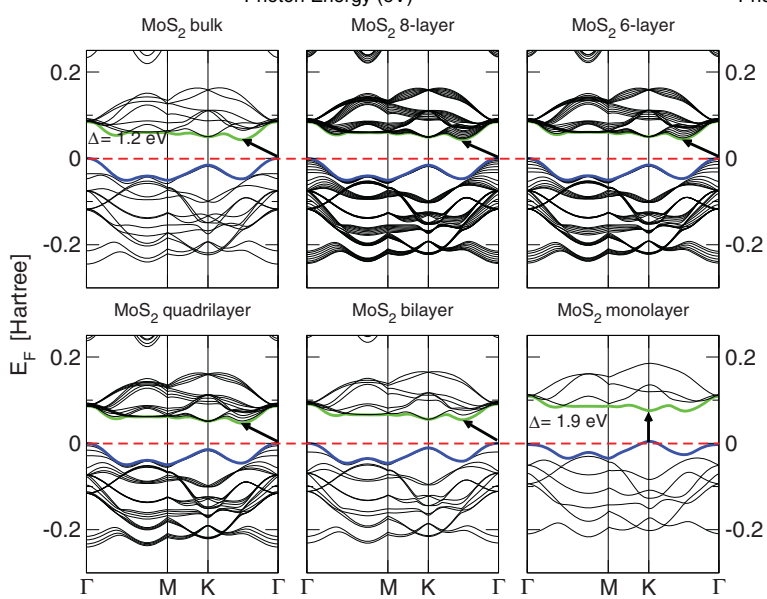
Applications
- THz detector
- Non-dissipative device
- Spintronics

Transition metal dichalcogenide (TMD)

MoS_2, $MoSe_2$, $MoTe_2$, WS_2, WSe_2, WTe_2,… (MX_2)



K. F. Mak et. al., Phys. Rev. Lett. 105, 136805 (2010)



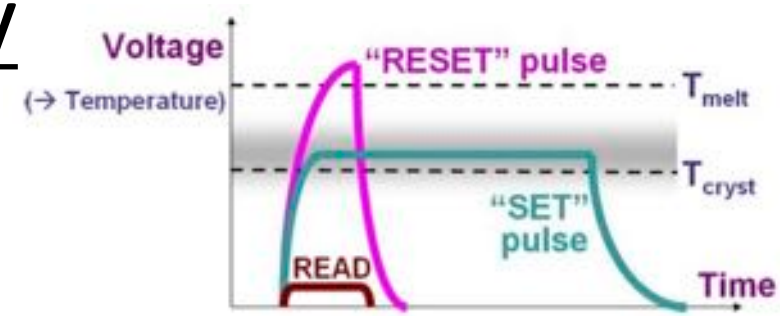
A. Kuc et. al., Phys. Rev. B, 83, 245213 (2011)

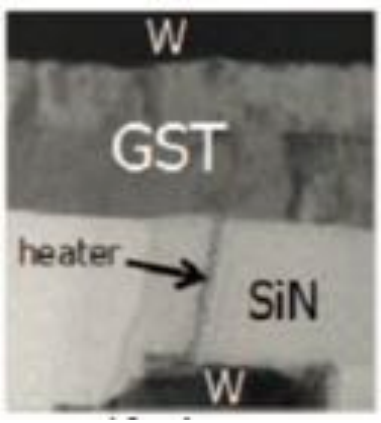
Phase change memory

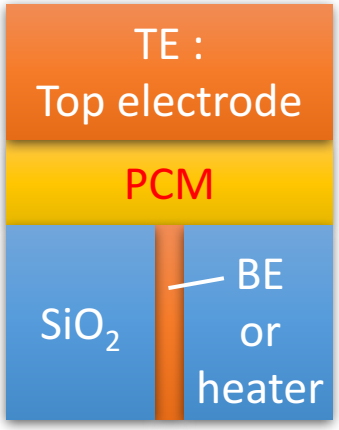
PCM (Phase Change Material)

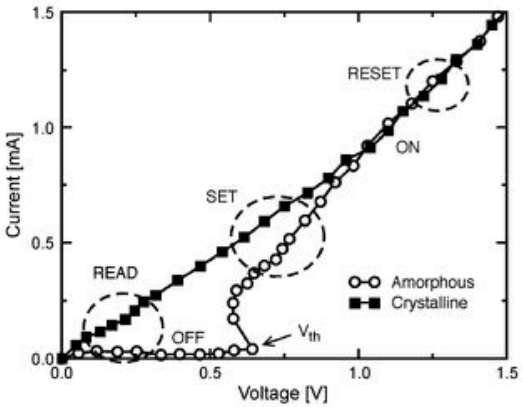
Chalcogenides

Ge-Sb-Te alloy ($GeTe-Sb_2Te_3$)



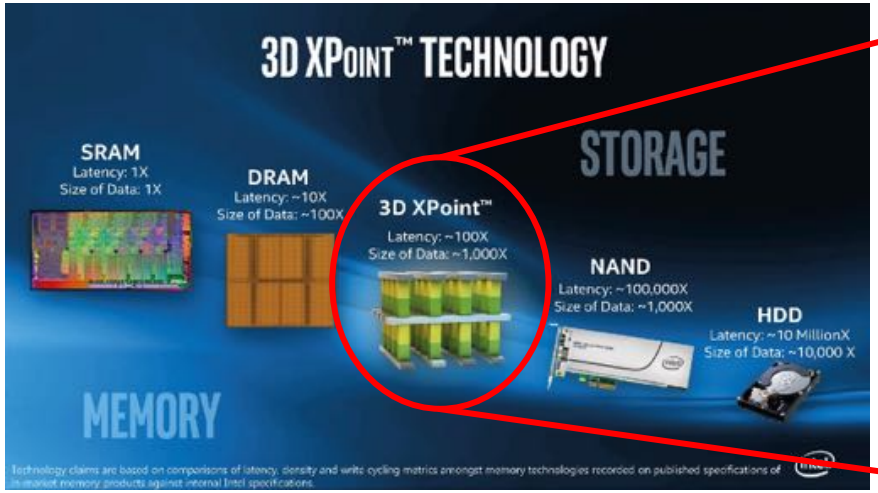




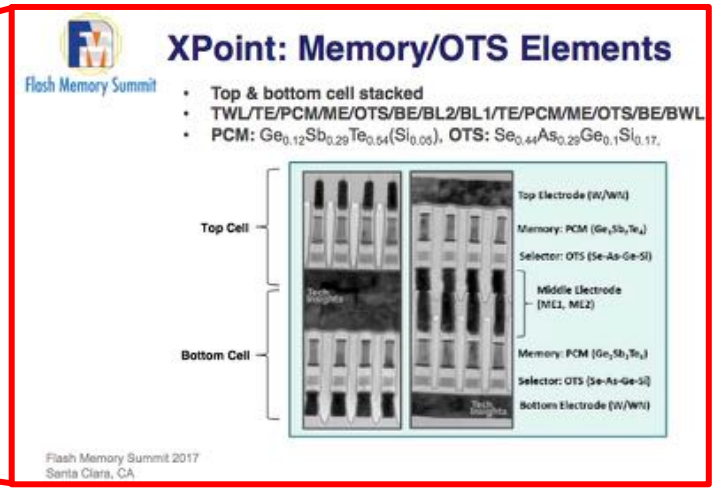


H.-S. P. Wong et al., *Proceedings of IEEE*, **98**, 2201 (2010)

G. W. Burr et al., *IEEE J. Emerg. Selected Topics in Circuit and Systems*, **6**, 146 (2016)



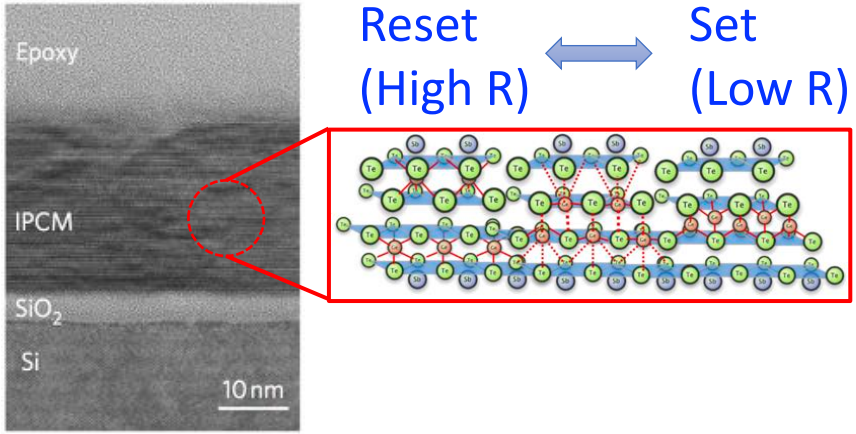
Intel and Micron

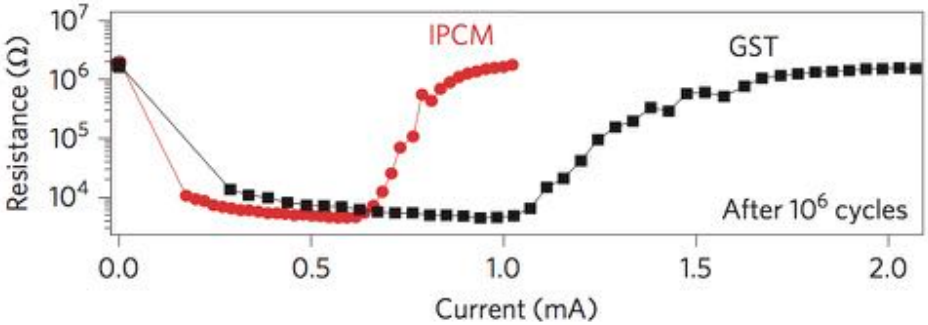


Tech Insights, Flash Memory Summit 2017

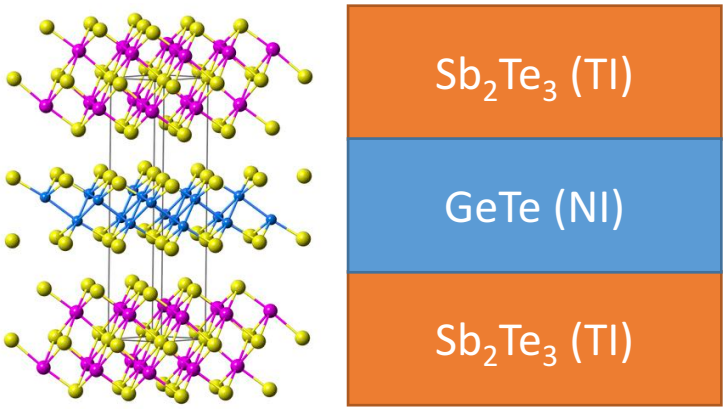
Chalcogenide superlattices for phase change memory

$GeTe/Sb_2Te_3$ superlattice





A. V. Kolobov et al., *Nat. Mater.* **3**, 703 (2004)
J. Tominaga et al., *Jap. J. Appl. Phys.* **47**, 5463 (2008)
R. E. Simpson et al., *Nat. Nanotech.* **6**, 501 (2011)



NI/TI stacking
TI : Topological insulator
NI : Normal insulator

Unusual electronic properties are expected.

Motivation

- Exploration of electronic structures of chalcogenide heterostructures.

$MoTe_2/Sb_2Te_3$ (TMDC/TI)
$GeTe/Sb_2Te_3$ (NI/TI, phase change memory)

Methods

- Density functional theory code: **WIEN2k***
- Functional: GGA-PBE or mBJ-LDA**
- Spin orbit coupling (soc)
- Geometry relaxation: DFT-D3 (Grimme)***

* K. Schwarz and P. Blaha. Comp. Mater. Sci. 28, 259 (2003).
** F. Tran and P. Blaha. Phys. Rev. Lett. 102, 226401 (2009).
*** S. Grimme. J. Comput. Chem. 25, 1463 (2004).

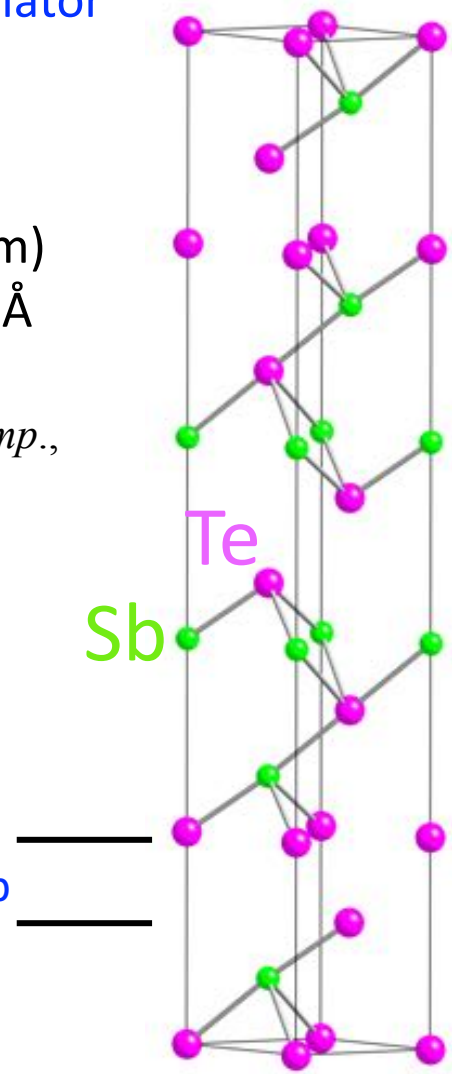
Band structure of Sb_2Te_3

Typical topological insulator

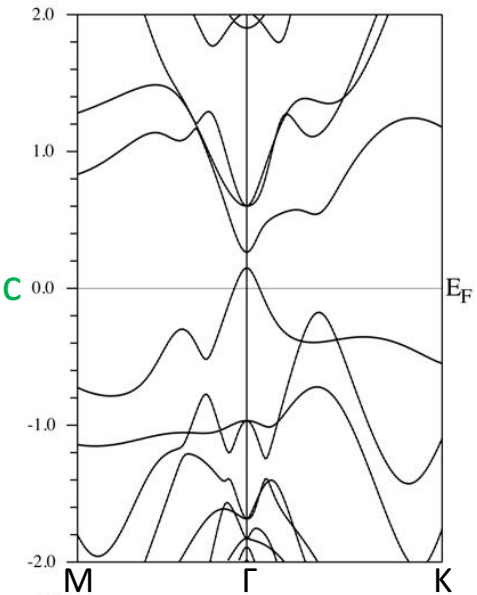
Bulk Sb_2Te_3

Space group : 166 (R-3m)
a = 4.262 Å, c = 30.435 Å

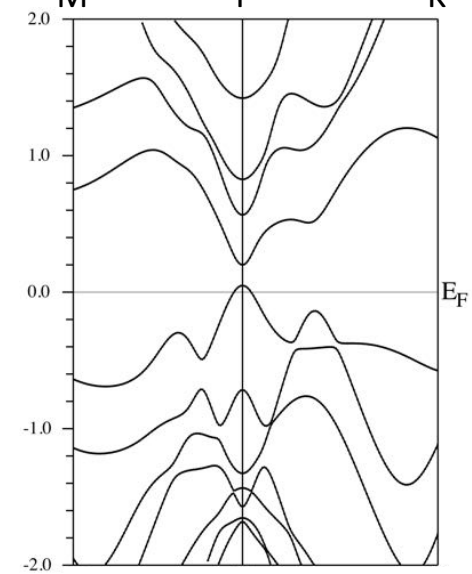
W.-S. Kim, *J. Alloys and Comp.*, **252**, 166 (1997)



without soc

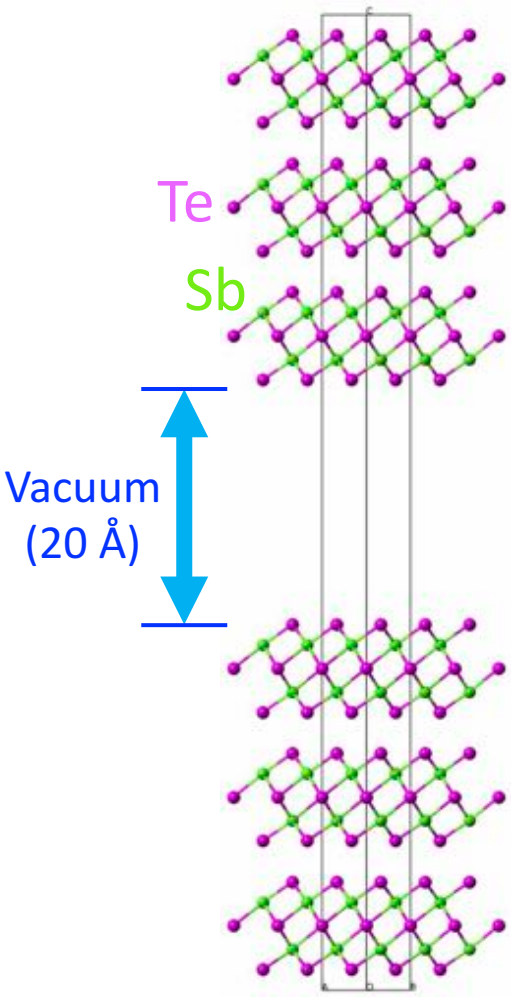


with soc

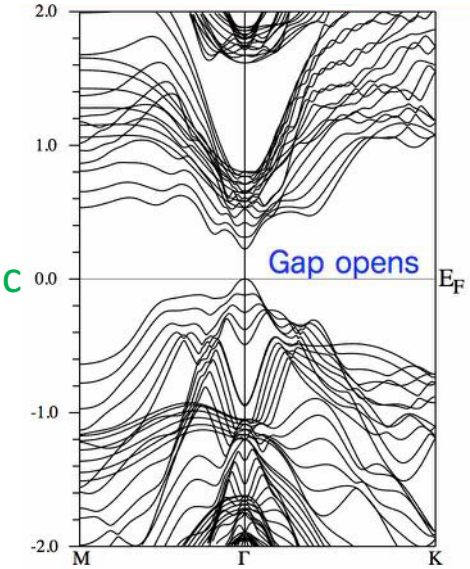


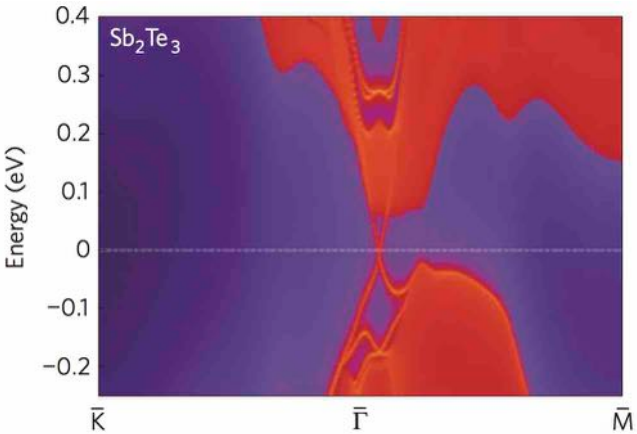
Band structure including vacuum slab

Sb_2Te_3-6QL-vacuum (20Å)
(QL: Quintuple layer)



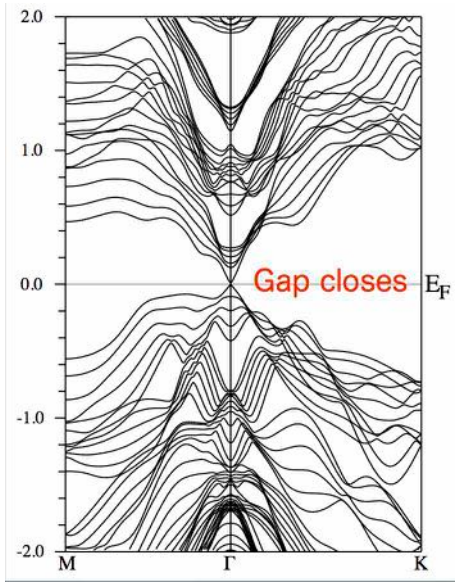
without soc

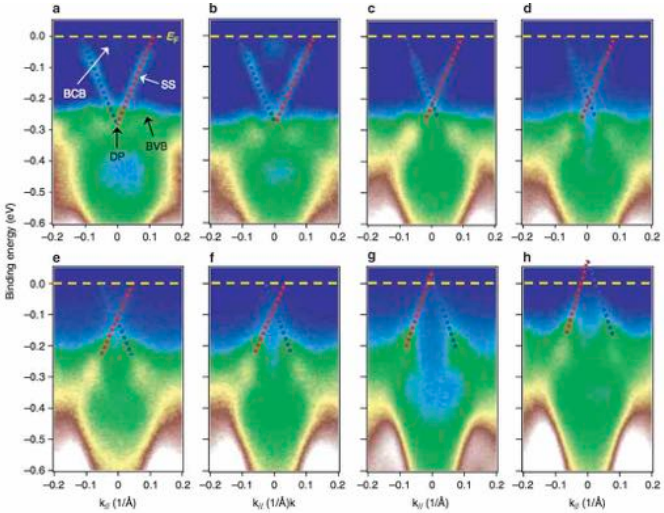




H. Zhang et al., *Nat. Phys.*, **5**, 438 (2009)

with soc





J. Zhang et al., *Nat. Comm.*, **2**, 574 (2011)

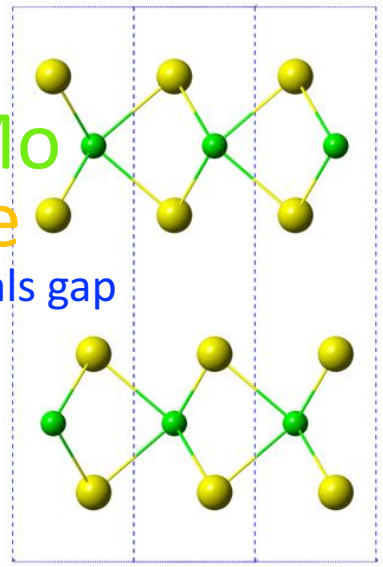
Dirac cone at the Γ point

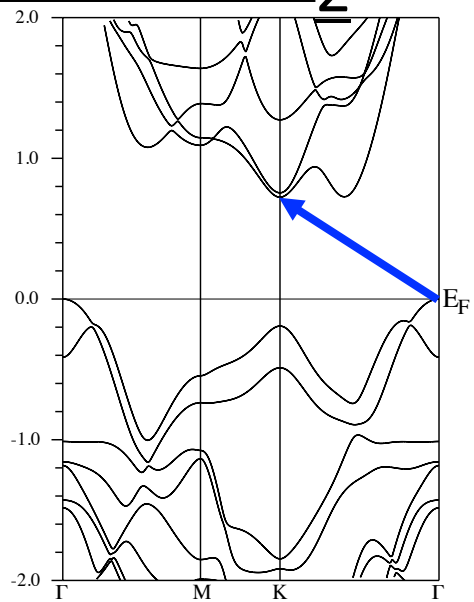
Band structures of $MoTe_2$

Bulk

Mo
Te

Van der Waals gap

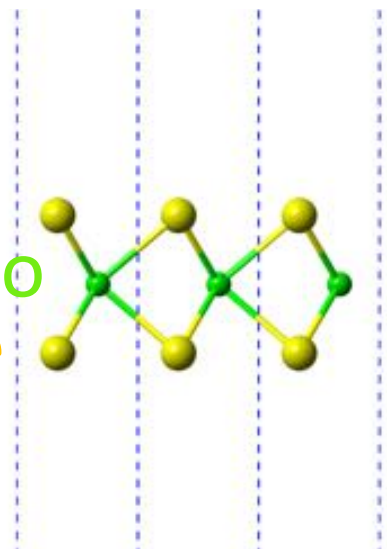


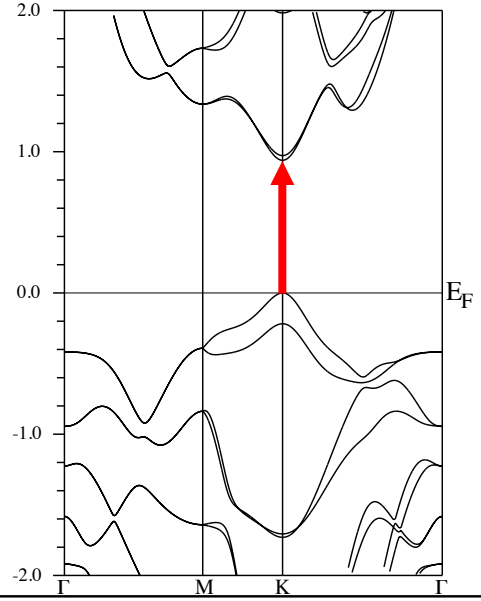


Indirect transition

Monolayer

Mo
Te

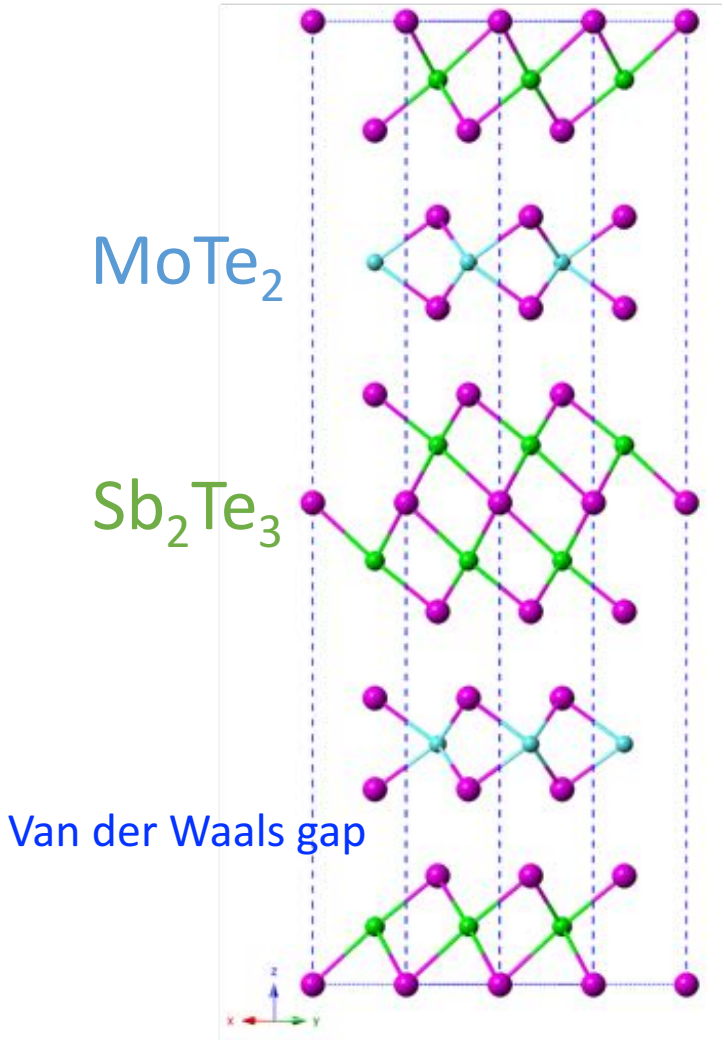


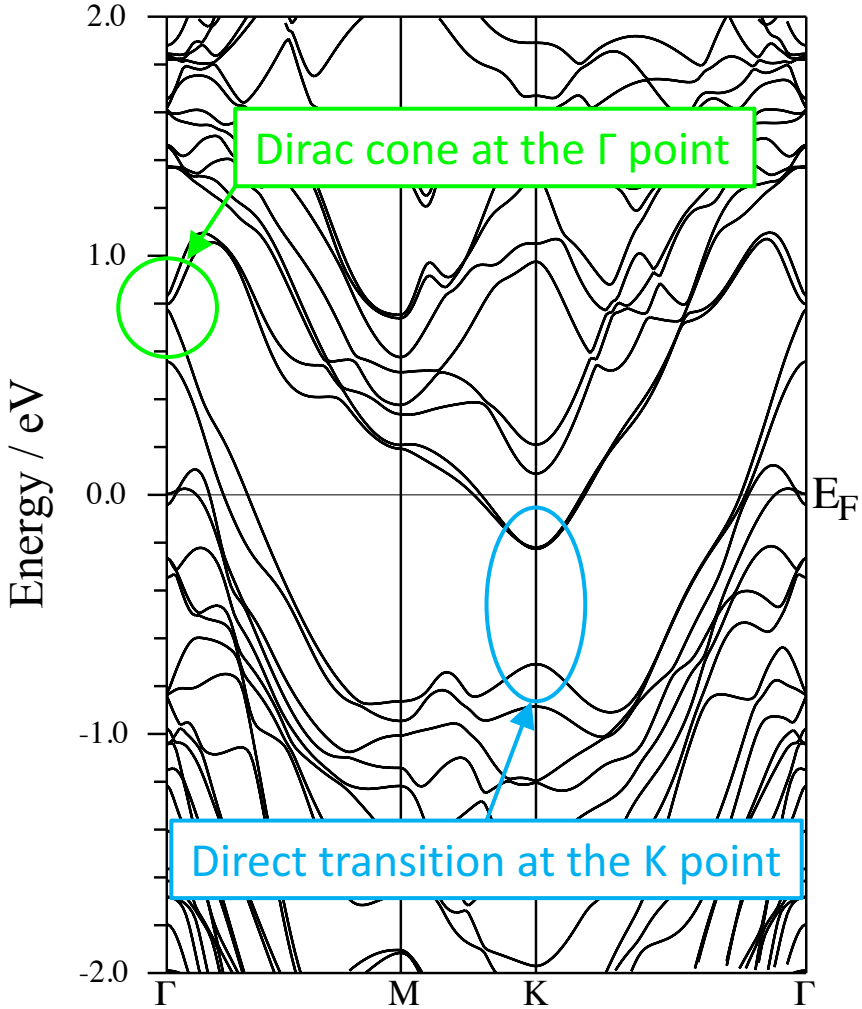


Direct transition

Transition at the K point

$MoTe_2/Sb_2Te_3$ heterostructure

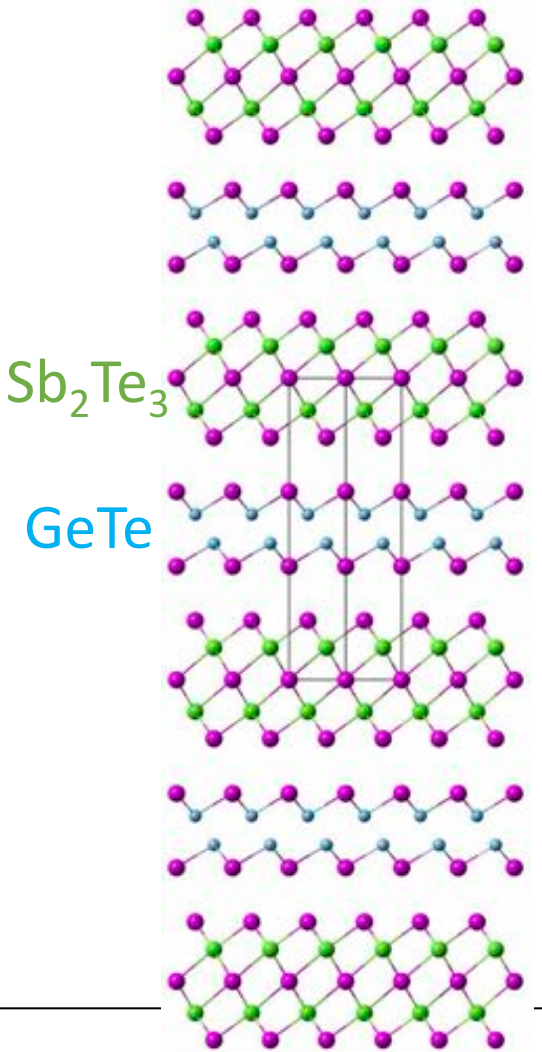


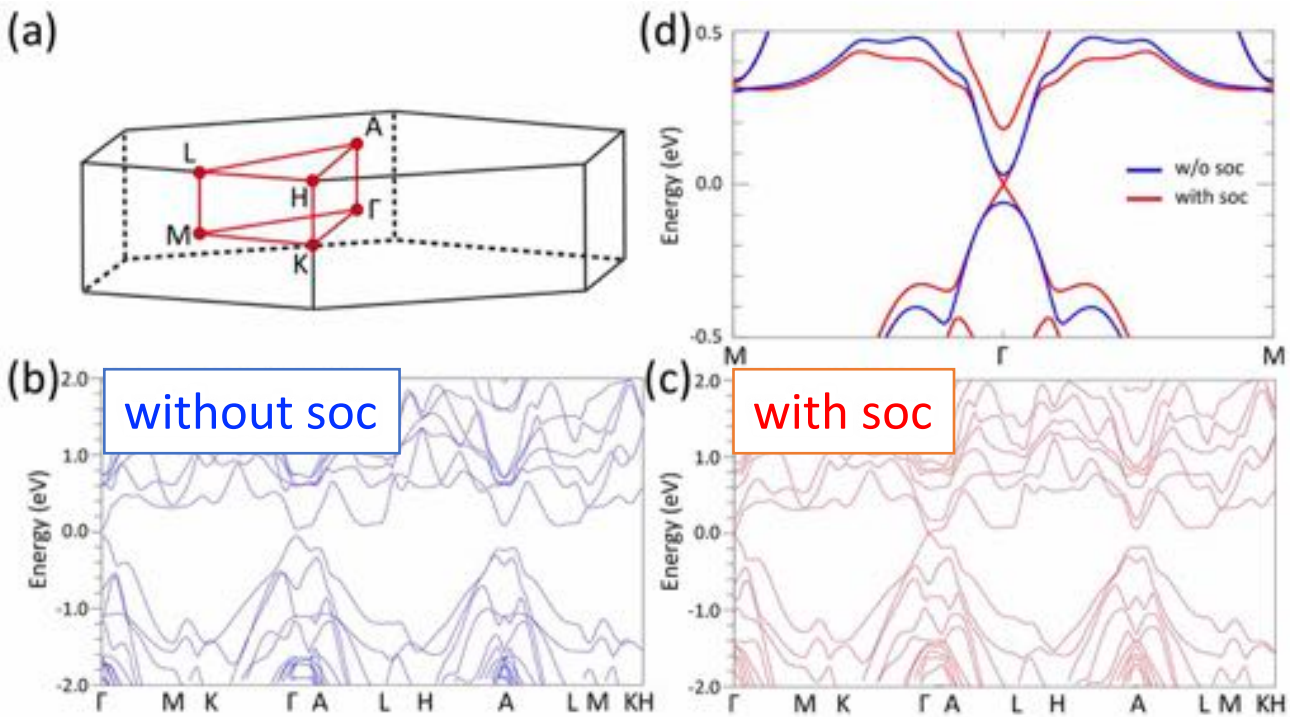


GeTe/Sb_2Te_3 heterostructure

GeTe : Normal insulator, Sb_2Te_3 : topological insulator

$(GeTe)_2/(Sb_2Te_3)_1$ superlattice



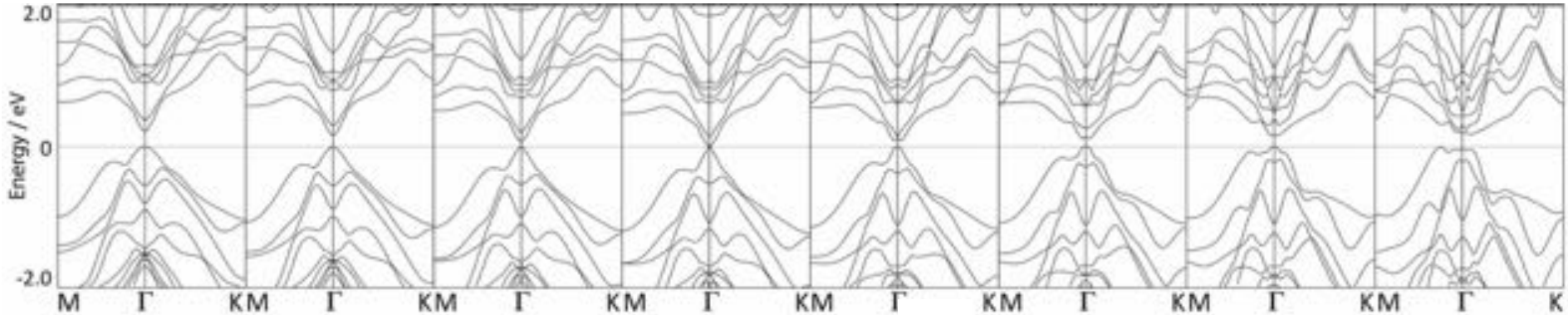


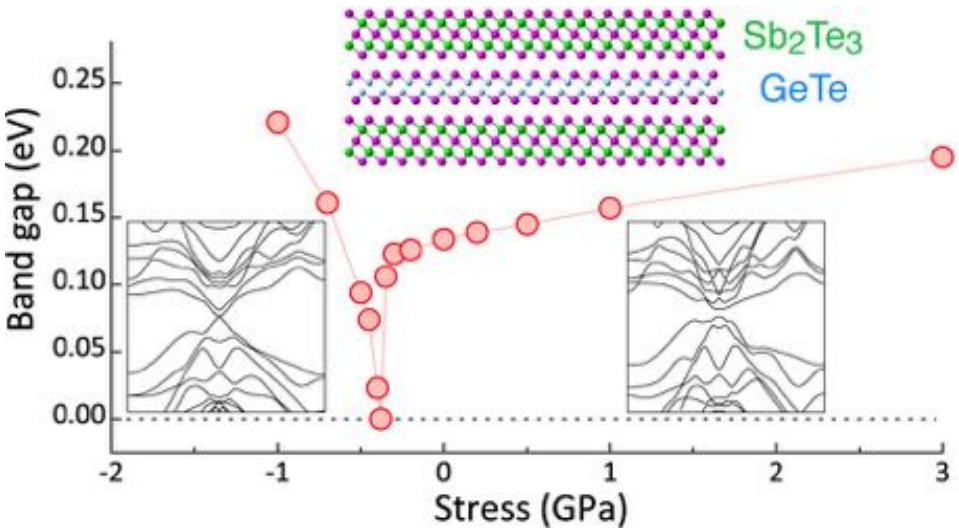
Y. Saito et al., *ACS Appl. Mater. Interfaces*, **9**, 23918 (2017)

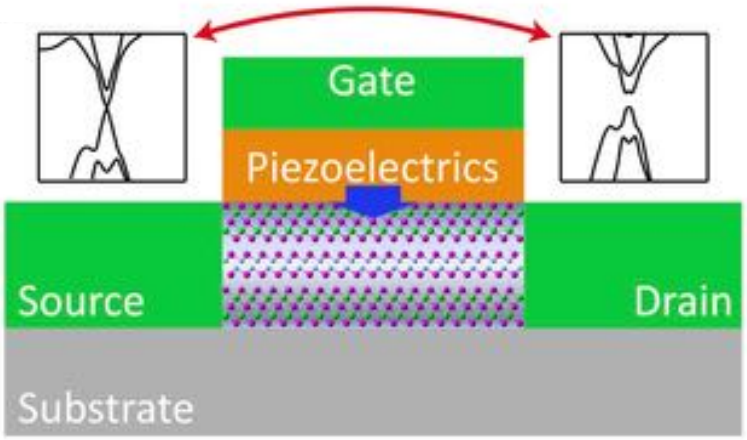
Band gap tuning

Tensile ← → **Stress** → **Compressive**

-1.0 GPa	-0.7 GPa	-0.45 GPa	-0.38 GPa	-0.3 GPa	0 GPa	1 GPa	3 GPa







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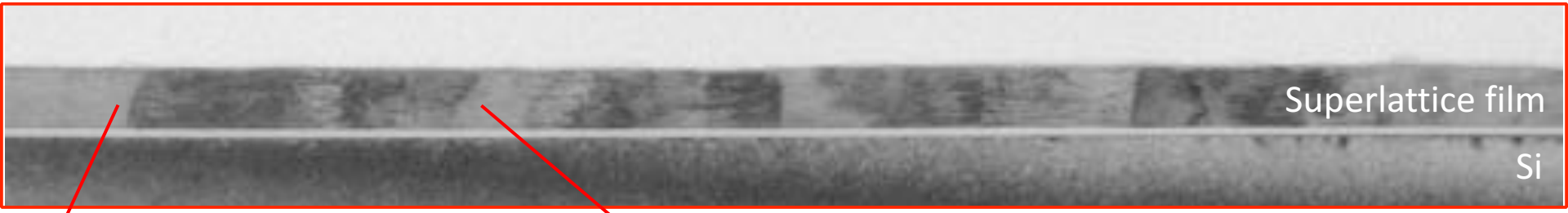
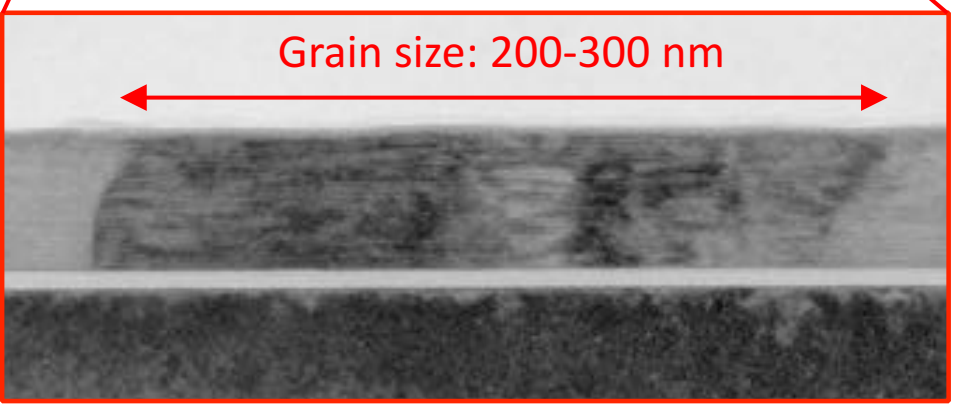
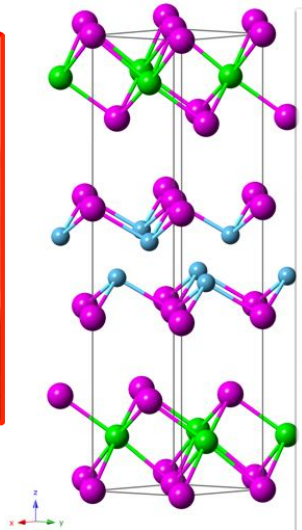
Fabrication of superlattice films

Sputter grown $GeTe/Sb_2Te_3$ superlattice film

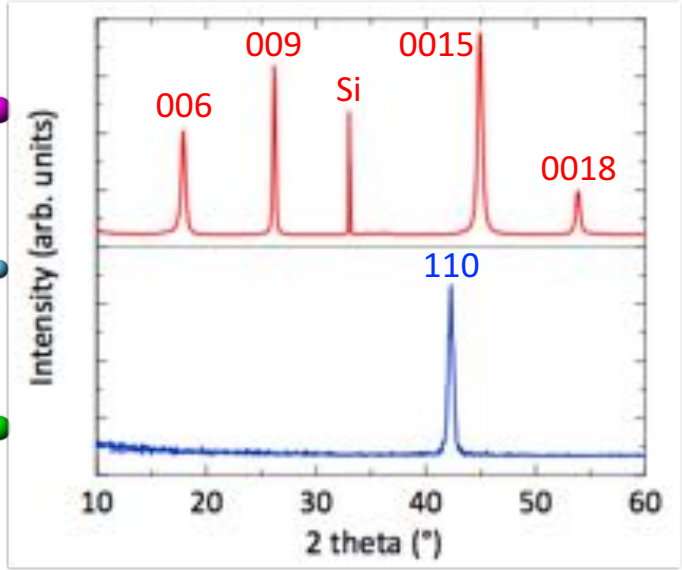
Cross-sectional TEM image





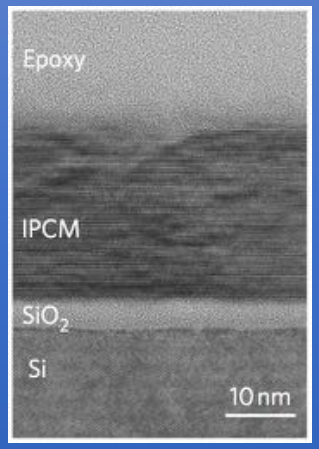


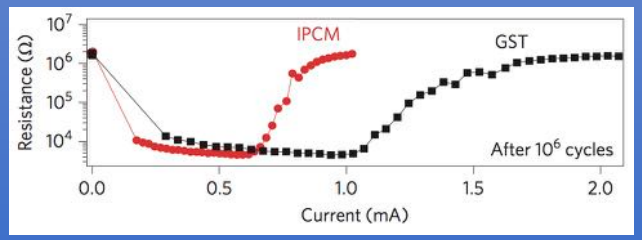
XRD (out-of-plane, in-plane)

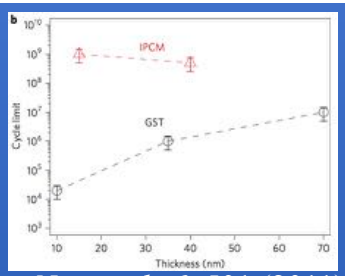


Applications

Phase change memory

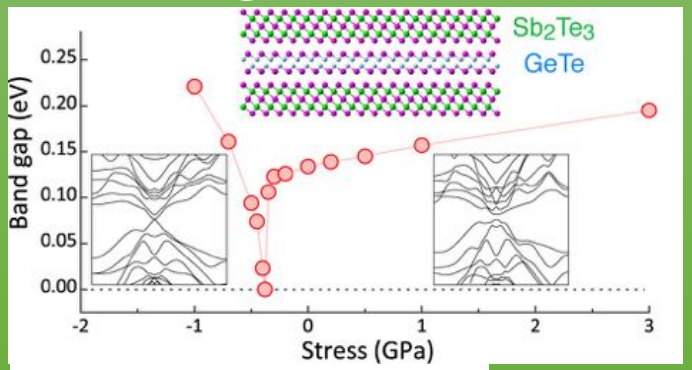


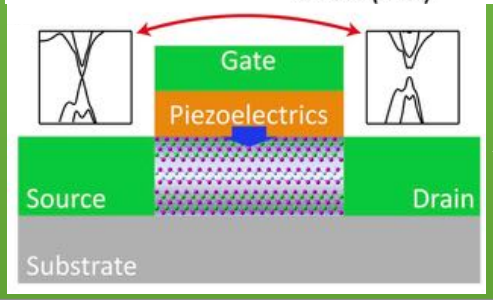




R. E. Simpson et al., *Nat. Nanotech.* **6**, 501 (2011)

Switching device





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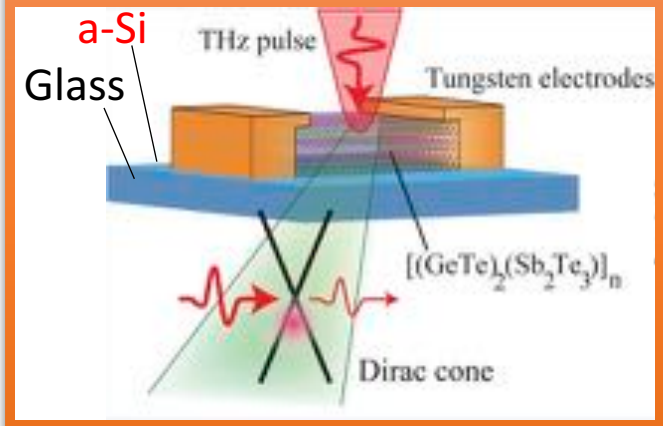
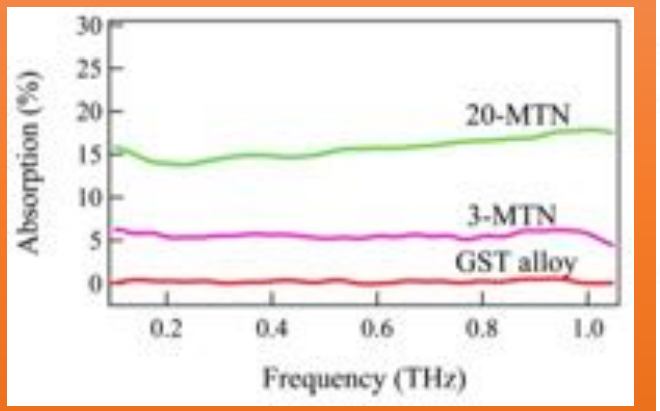
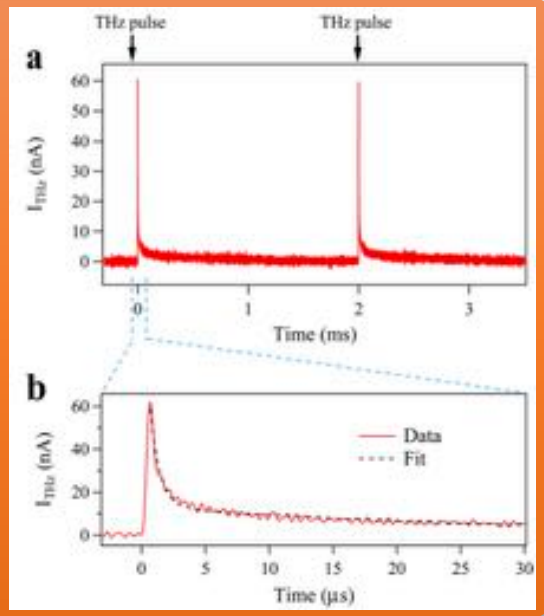
THz detector







K. Makino et al., *ACS Appl. Mater. Interfaces*, **8**, 32408 (2016)

Summary

- $MoTe_2/Sb_2Te_3$ heterostructure possesses both features of transition metal dichalcogenide and topological insulator. However, a large difference of band alignment makes difficult to harness their properties.

- $GeTe/Sb_2Te_3$ heterostructure is promising not only for phase change memory but also for novel electronic devices that exploit topological insulator properties.

Thank you for your attention!

Acknowledgement
This work was supported by CREST, JST (No. JPMJCR14F1) and by JSPS KAKENHI Grant Nos. 26886015 and 16K04896, Japan.