

Supplementary information

Vibrational Spectra of $\text{Pb}_2\text{Bi}_2\text{Te}_3$, PbBi_2Te_4 and PbBi_4Te_7 Topological Insulators: Temperature Dependent Raman and Theoretical Insight from DFT Simulations

Privanath Mal^a, G. Bera^a, G. R. Turpu^a, Sunil K. Srivastava^b, A. Gangan^c, Brahmananda Chakraborty^{*c}, Bipul Das^d and Pradip Das^{*a}

^a Department of Pure Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur-495009, India.
E-mail: pradipd.iitb@gmail.com

^b Department of Physics, Mahtma Gandhi Central University, East Champaran, Motihari, Bihar-845401, India.

^c High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai-40008, India.

E-mail: brahma@barc.gov.in

^d Department of Physics, National Changhua University of Education, Jin-De Road, Changhua 500, Taiwan.

Entry	Content	Page no.
01	Thickness	S2
02	EDAX	S3
03	Band structure	S4
04	Phonon dispersion	S5
05	Character table	S6-S7

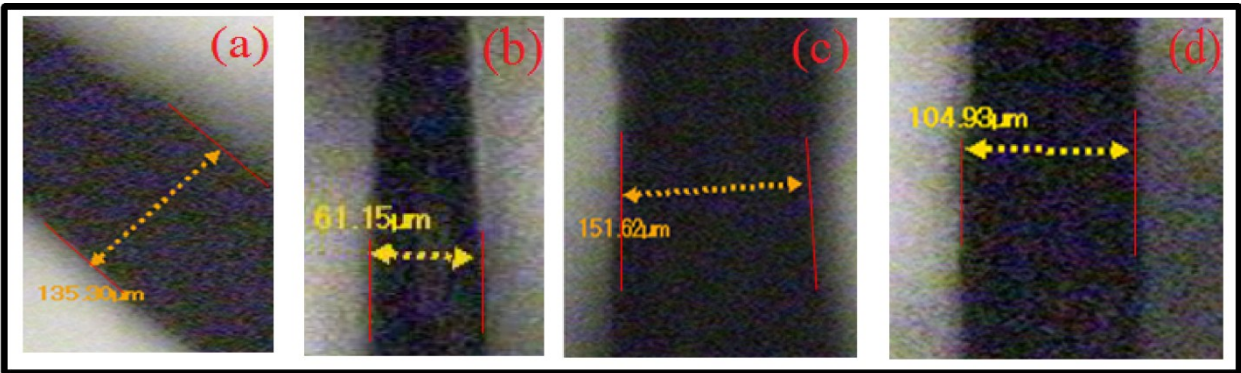
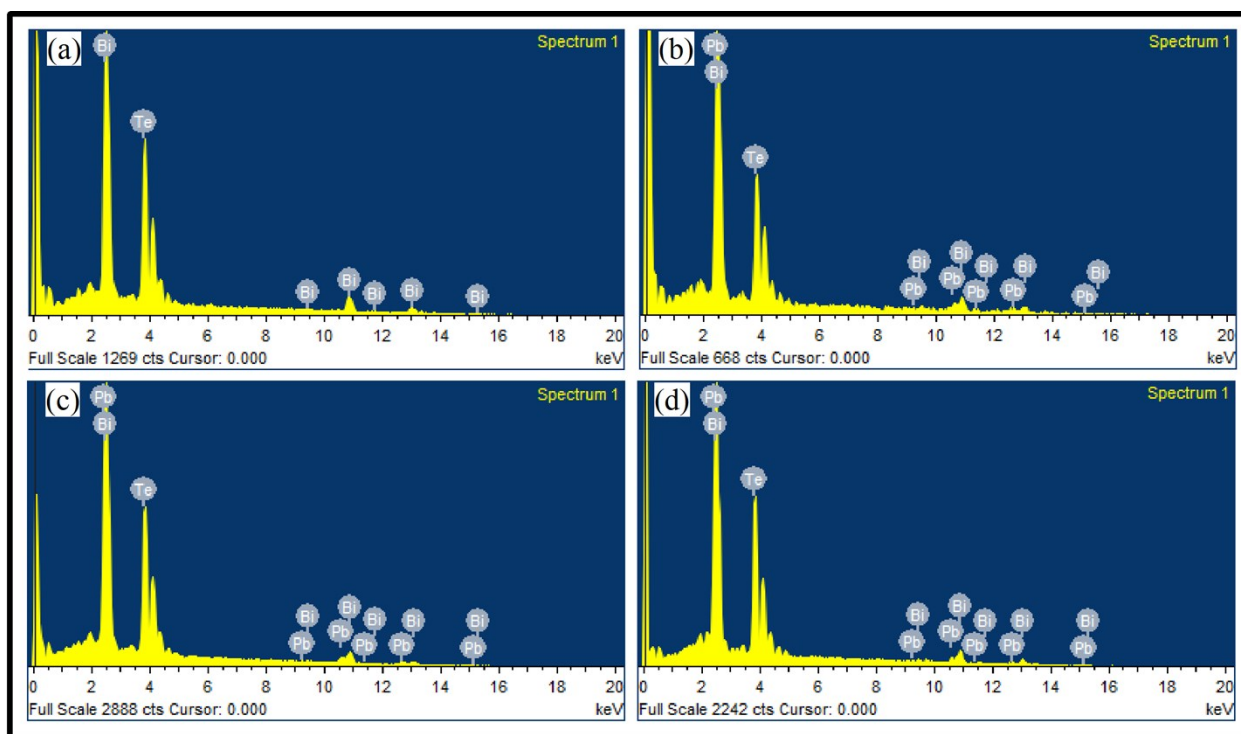


Fig. S1 Thickness of (a) Bi₂Te₃, (b) Pb₂Bi₂Te₃, (c) PbBi₂Te₄ and (d) PbBi₄Te₇ single crystal flakes measured through optical microscope.



Specimen	Weight (%)	
	Theoretical	Experimental
Bi ₂ Te ₃	Bi: 52.19	Bi: 52.25
	Te: 47.80	Te: 47.75
Pb ₂ Bi ₂ Te ₃	Pb: 34.10	Pb: 33.83
	Bi: 34.40	Bi: 34.43

	Te: 31.49	Te: 31.74
PbBi ₂ Te ₄	Pb: 19.31 Bi: 36.57 Te: 45.11	Pb: 19.31 Bi: 35.73 Te: 44.96
PbBi ₄ Te ₇	Pb: 10.70 Bi: 43.17 Te: 46.12	Pb: 10.11 Bi: 43.16 Te: 46.73

Fig. S2 EDAX spectra for (a) Bi₂Te₃, (b) Pb₂Bi₂Te₃, (c) PbBi₂Te₄ and (d) PbBi₄Te₇ single crystal flakes.

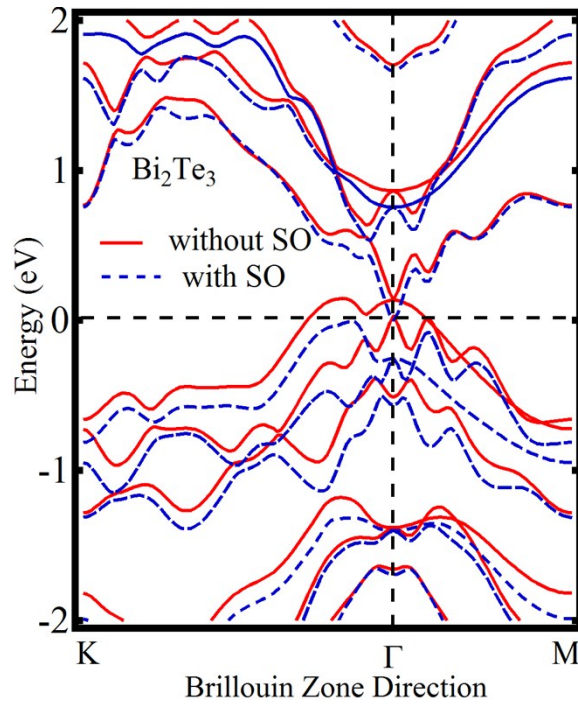


Fig. S3 Band structure of Bi₂Te₃ with and without spin-orbit interactions; the band structure of Bi₂Te₃ film is resolved correctly when including spin-orbit effect and the Dirac cone is observed at the Γ point in the Brillouin zone.

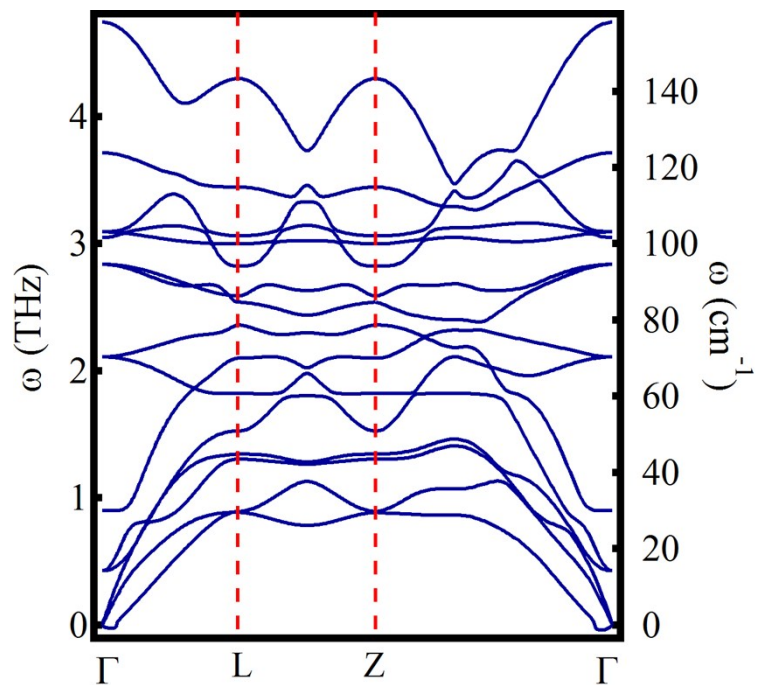


Fig. S4 Phonon frequencies of Bi₂Te₃ in the Brillouin zone direction; there are no negative frequencies which reflect the stability.

Character table

1. Bi_2Te_3

point group $D_{3d} (-3m)$
there are 6 classes
the character table:

	E	2C3	3C2'	i	2S6	3s _d
A _{1g}	1.00	1.00	1.00	1.00	1.00	1.00
A _{2g}	1.00	1.00	-1.00	1.00	1.00	-1.00
E _g	2.00	-1.00	0.00	2.00	-1.00	0.00
A _{1u}	1.00	1.00	1.00	-1.00	-1.00	-1.00
A _{2u}	1.00	1.00	-1.00	-1.00	-1.00	1.00
E _u	2.00	-1.00	0.00	-2.00	1.00	0.00

Mode symmetry, $D_{3d} (-3m)$ point group:

freq (1 - 1) =	3.5	[cm-1]	--> A _{2u} L ₂ '	I
freq (2 - 3) =	8.0	[cm-1]	--> E _u L ₃ '	I
freq (4 - 5) =	38.1	[cm-1]	--> E _g L ₃	R
freq (6 - 6) =	56.3	[cm-1]	--> A _{1g} L ₁	R
freq (7 - 8) =	63.7	[cm-1]	--> E _u L ₃ '	I
freq (9 - 10) =	97.4	[cm-1]	--> E _u L ₃ '	I
freq (11 - 11) =	102.5	[cm-1]	--> A _{2u} L ₂ '	I
freq (12 - 13) =	105.1	[cm-1]	--> E _g L ₃	R
freq (14 - 14) =	127.5	[cm-1]	--> A _{2u} L ₂ '	I
freq (15 - 15) =	135.9	[cm-1]	--> A _{1g} L ₁	R

2. PbBi_4Te_7

point group $D_{3d} (-3m)$

there are 6 classes
the character table:

	E	2C3	3C2'	i	2S6	3s _d
A _{1g}	1.00	1.00	1.00	1.00	1.00	1.00
A _{2g}	1.00	1.00	-1.00	1.00	1.00	-1.00
E _g	2.00	-1.00	0.00	2.00	-1.00	0.00
A _{1u}	1.00	1.00	1.00	-1.00	-1.00	-1.00
A _{2u}	1.00	1.00	-1.00	-1.00	-1.00	1.00
E _u	2.00	-1.00	0.00	-2.00	1.00	0.00

Mode symmetry, D_{3d} (-3m) point group:

freq (1 - 2) =	-4.8	[cm-1]	--> E _u L ₃ '	I
freq (3 - 3) =	-2.2	[cm-1]	--> A _{2u} L ₂ '	I
freq (4 - 5) =	6.1	[cm-1]	--> E _u L ₃ '	I
freq (6 - 6) =	9.4	[cm-1]	--> A _{2u} L ₂ '	I
freq (7 - 8) =	19.9	[cm-1]	--> E _g L ₃	R
freq (9 - 10) =	34.2	[cm-1]	--> E _u L ₃ '	I
freq (11 - 12) =	36.3	[cm-1]	--> E _g L ₃	R
freq (13 - 13) =	37.9	[cm-1]	--> A _{1g} L ₁	R
freq (14 - 14) =	53.8	[cm-1]	--> A _{1g} L ₁	R
freq (15 - 16) =	59.3	[cm-1]	--> E _u L ₃ '	I
freq (17 - 18) =	68.6	[cm-1]	--> E _u L ₃ '	I
freq (19 - 19) =	75.2	[cm-1]	--> A _{2u} L ₂ '	I
freq (20 - 21) =	77.6	[cm-1]	--> E _g L ₃	R
freq (22 - 23) =	91.8	[cm-1]	--> E _u L ₃ '	I
freq (24 - 25) =	93.0	[cm-1]	--> E _g L ₃	R
freq (26 - 27) =	98.1	[cm-1]	--> E _u L ₃ '	I
freq (28 - 29) =	103.9	[cm-1]	--> E _g L ₃	R
freq (30 - 30) =	109.2	[cm-1]	--> A _{2u} L ₂ '	I
freq (31 - 31) =	110.4	[cm-1]	--> A _{1g} L ₁	R
freq (32 - 32) =	113.3	[cm-1]	--> A _{2u} L ₂ '	I
freq (33 - 33) =	136.9	[cm-1]	--> A _{2u} L ₂ '	I
freq (34 - 34) =	139.0	[cm-1]	--> A _{2u} L ₂ '	I
freq (35 - 35) =	139.2	[cm-1]	--> A _{1g} L ₁	R
freq (36 - 36) =	142.5	[cm-1]	--> A _{1g} L ₁	R