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Lattice dynamics of Bi_2Se_3 at high pressures

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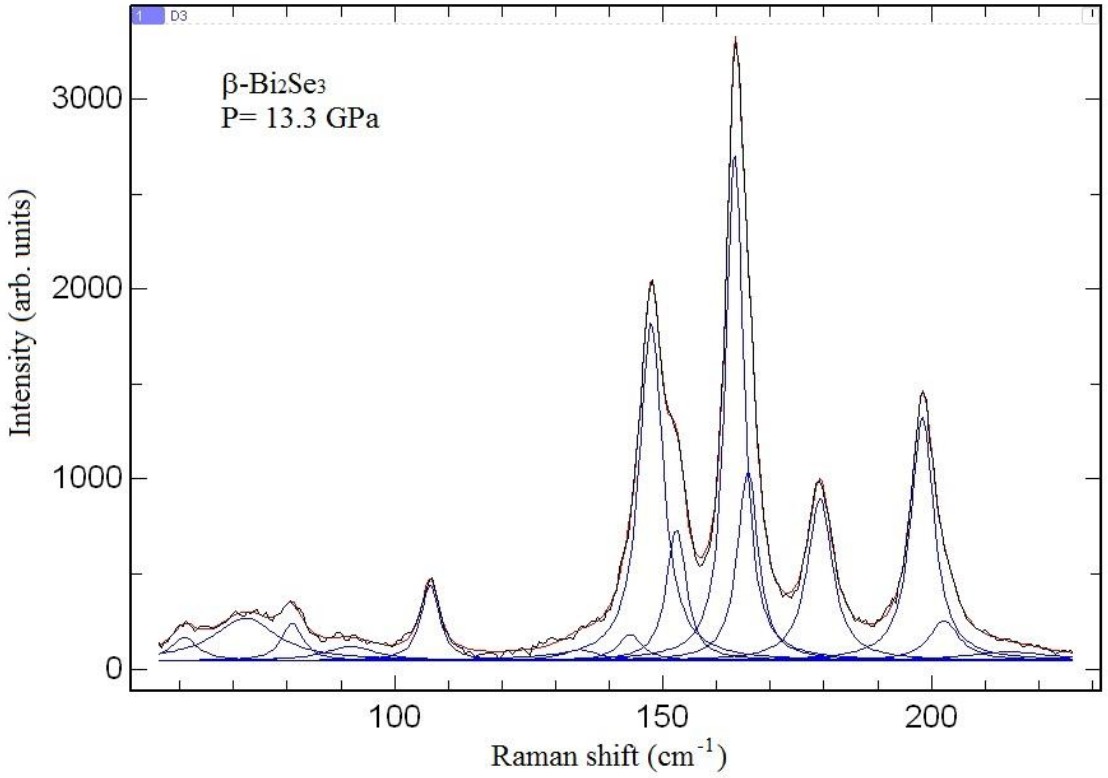
Supplementary materials

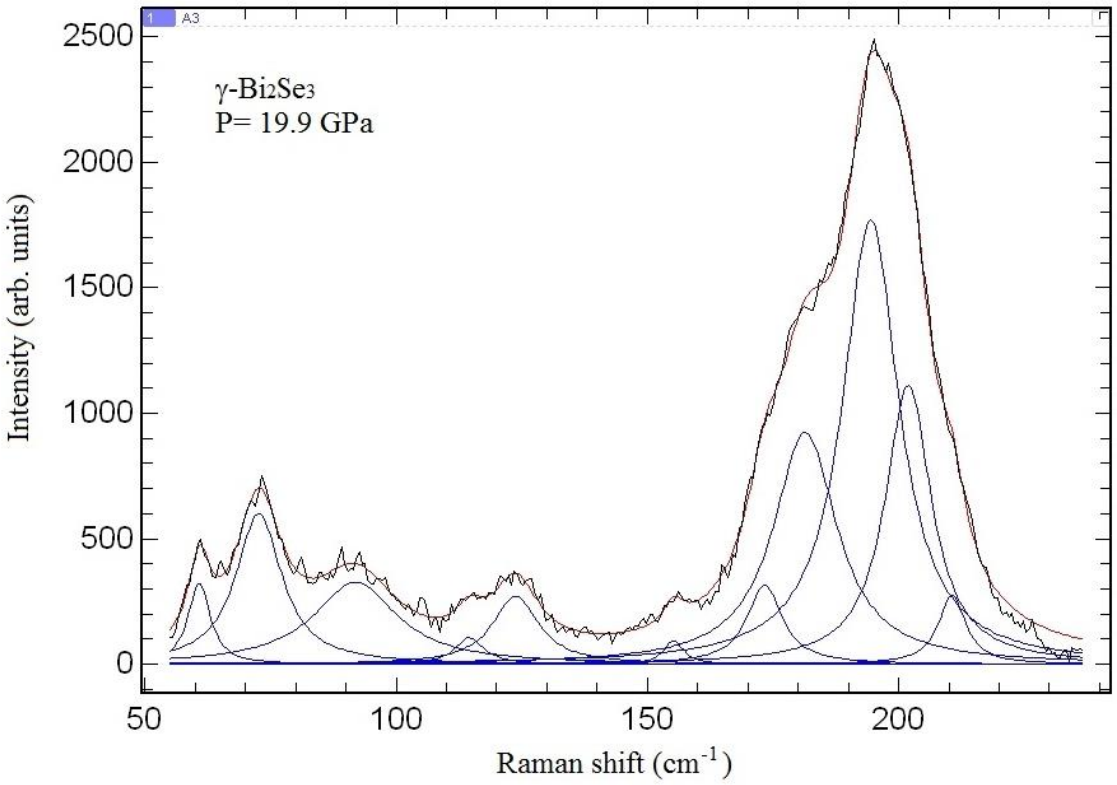
Supplementary Figure 1.

Spectrum of β-Bi_2Te_3 at 13.3 GPa and the corresponding fit of Voigt profiles corresponding to the Raman-active modes of the C2/m structure.



Supplementary Figure 2.

Spectrum of γ-Bi_2Te_3 at 19.9 GPa and the corresponding fit of Voigt profiles corresponding to the Raman-active modes of the C2/c structure.



Supplementary Table I. Theoretical (th.) *ab initio* IR-mode frequencies and pressure coefficients in α-Bi_2Te_3 (R-3m phase) at room temperature and P_0= 1 atm, as

obtained from fits to the data using $\omega(P) = \omega(P_0) + a_1 \cdot (P - P_0)$. Experimental (exp.) and theoretical IR-mode frequencies at room pressure of other works are given for comparison.

Mode	ω_0(th.) (cm^{-1})	a_1(th.) (cm^{-1}/GPa)	ω_0 (th.) (cm^{-1})	ω_0 (th.) (cm^{-1})	ω_0 (th.) (cm^{-1})	ω_0 (exp.) (cm^{-1})	ω_0 (exp.) (cm^{-1})
E_u^1	58.9	3.14	48.4	63.2	71.1	50	-
E_u^2	95.4	1.23	91.2	97.4	93.5	94	-
A_{2u}^1	99.2	2.59	95.1	102.6	116.4	95	-
A_{2u}^2	120.5	1.82	118.6	127.9	141.3	120	120
Ref.	This work	This work	1[a]	1[b]	2	3	4

a GGA calculations including the spin-orbit coupling.
b GGA calculations without the spin-orbit coupling.

It can be observed that the room pressure frequencies of our calculations without spin-orbit coupling and using GGA-PBEsol compare reasonably well with experimental values and are intermediate between the theoretical results obtained using GGA with and without spin-orbit coupling (see Ref. 1). Our theoretical values are considerably better than the values reported in Ref. 2 obtained from a Born-von Karman model.

Supplementary Table II. Theoretical (th.) *ab initio* IR-mode frequencies and pressure coefficients observed in β-Bi_2Te_3 (C2/m phase) at room temperature at P_0= 9.2 GPa as obtained from fits using $\omega(P) = \omega(P_0) + a_1 \cdot (P-P_0)$.

Mode	ω (P_0) (th.) (cm^{-1})	a_1 (th.) (cm^{-1}/GPa)
B_u^1	51.9	1.02
A_u^1	56.0	0.91
B_u^2	73.5	1.20
A_u^2	87.8	1.69
B_u^3	93.9	1.50
B_u^4	97.7	1.95
A_u^3	99.9	0.83
A_u^4	122.6	1.16
B_u^5	124.0	1.28
B_u^6	124.9	2.22
B_u^7	136.1	1.69
B_u^8	147.4	2.40

Supplementary Table III. Theoretical (th.) *ab initio* IR-mode frequencies and pressure coefficients observed in γ-Bi_2Te_3 (C2/c phase) at room temperature at P_0= 15.5 GPa as obtained from fits using $\omega(P) = \omega(P_0) + a_1 \cdot (P-P_0)$.

Mode	$\omega(P_0)$ (th.) (cm^{-1})	a_1 (th.) (cm^{-1}/GPa)
A_u^1	44.3	1.00
B_u^1	43.8	0.16
B_u^2	74.9	0.64
A_u^2	75.2	0.25
A_u^3	80.8	0.56
B_u^3	112.5	1.72
A_u^4	119.1	1.13
B_u^4	122.3	1.72
B_u^5	126.5	2.20
A_u^5	146.3	1.72
B_u^6	151.5	2.73
A_u^6	153.5	1.93

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