

Lattice dynamics of Bi₂Te₃ at high pressures

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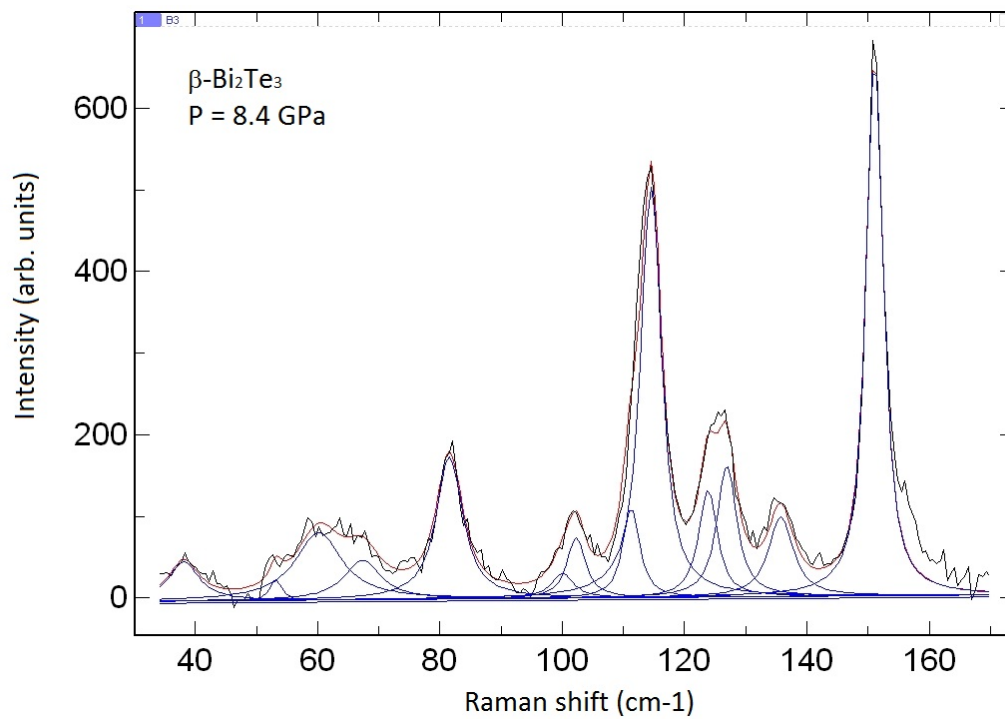
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Supplementary materials

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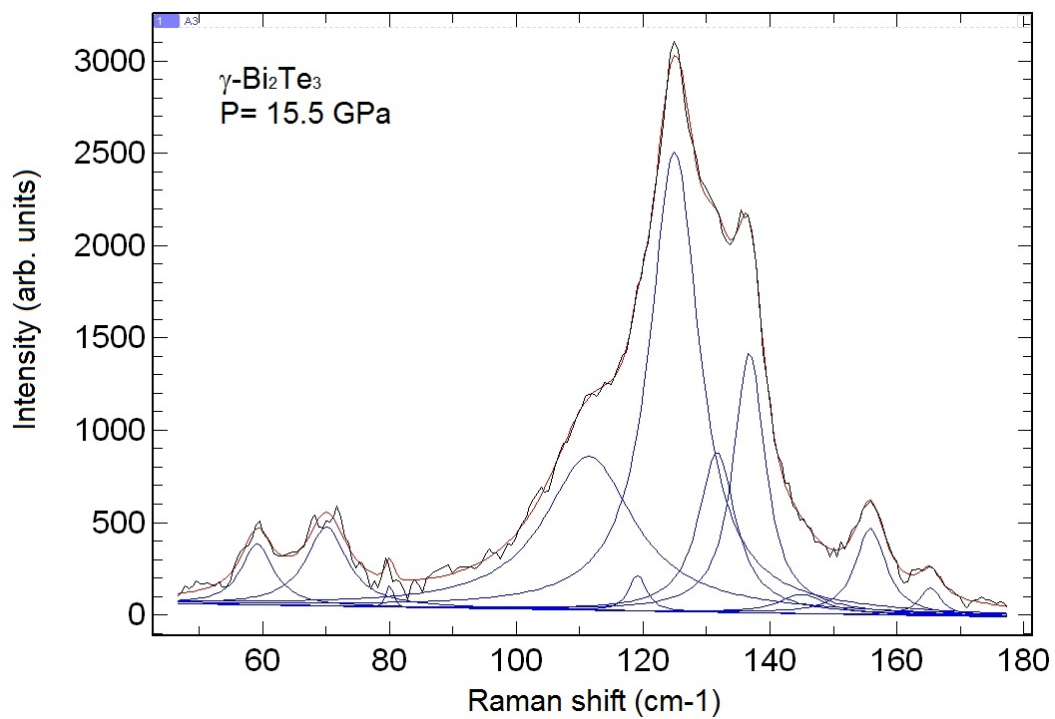
Supplementary Figure 1.

Spectrum of β -Bi₂Te₃ at 8.4 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 -Bi₂Te₃ at 15.5 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 -Bi₂Te₃ (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 -Bi₂Te₃ (C2/m phase) at room temperature at $P_0= 8.4$ 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)
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 -Bi₂Te₃ (C2/c phase) at room temperature at P₀= 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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