

Sample Preparation

The elements Bi, Sb and Te were evaporated from standard thermal effusion cells. The alternating element layers were deposited using the cell shutters. The element layer thickness was controlled by the shutter opening time while the molecular beam flux from each cell was maintained at a constant value, determined with a beam flux monitor. The growth rate at the respective molecular flux was determined before the deposition process. During growth, the beam flux was checked once and re-adjusted if deviations from the defined value occurred. Shutter opening times were in the orders of 1-2 seconds for the ~ 0.2 nm element layer thickness and scaled accordingly for thicker element layers.

BaF₂ substrates were cleaved from 10 mm × 10 mm bars from supplier Crystek.

Results of Rietveld refinements

Sample	BT-Q	BT-B1	BT-B2	BT-B3
Crystal system	Rhombohedral			
Space group	$R\bar{3}m$			
Volume	510.07 (9)	510.02 (9)	508.04 (7)	508.50 (9)
Z	3			
Density (calculated)	7.82 gm cm ⁻³	7.82 gm cm ⁻³	7.85 gm cm ⁻³	7.85 gm cm ⁻³
Bi x, y, z U_{iso}	0, 0, 0.4000 (1) 0.032 (2) Å ²	0, 0, 0.3997 (1) 0.039 (1) Å ²	0, 0, 0.3997 (1) 0.062 (2) Å ²	0, 0, 0.4013 (1) 0.036 (6)
Te1 x, y, z U_{iso}	0, 0, 0.2099 (1) 0.032 (2) Å ²	0, 0, 0.2088 (1) 0.019 (1) Å ²	0, 0, 0.2108 (1) 0.077 (2) Å ²	0, 0, 0.2089 (1) 0.019 (8) Å ²
Te2 x, y, z U_{iso}	0, 0, 0 0.036 (3) Å ²	0, 0, 0 0.038 (2) Å ²	0, 0, 0 0.077 (2) Å ²	0, 0, 0 0.019 (8) Å ²
No. of reflections	324	321	321	324
No. of profile points used	4098	2846	2838	2980
No. of Variables	88	93	84	85
R-factors ^a				
R _{wp}	0.0854	0.0523	0.0644	0.0848
R _p	0.0628	0.0383	0.0464	0.0566

^a. for definition of R-factors see reference [44].

Sample	ST-Q	ST-B1	ST-B2	ST-B3
Crystal system	Rhombohedral			
Space group	$R\bar{3}m$			
Volume	479.59 (2)	479.20 (6)	479.23 (6)	479.26 (4)
Z	3			
Density (calculated)	6.51 gm cm ⁻³	6.51 gm cm ⁻³	6.51 gm cm ⁻³	6.51 gm cm ⁻³
Sb x, y, z U_{iso}	0, 0, 0.3987 (1) 0.019 (1) Å ²	0, 0, 0.3979 (1) 0.054 (1) Å ²	0, 0, 0.4026 (1) 0.065 (2) Å ²	0, 0, 0.3996 (1) 0.020 (1)
Te1 x, y, z U_{iso}	0, 0, 0.2122 (1) 0.011 (1) Å ²	0, 0, 0.2163 (1) 0.062.(1) Å ²	0, 0, 0.2136 (1) 0.036 (2) Å ²	0, 0, 0.2145 (1) 0.023 (1) Å ²
Te2 x, y, z U_{iso}	0, 0, 0 0.011 (1) Å ²	0, 0, 0 0.062.(1)Å ²	0, 0, 0 0.036 (2) Å ²	0, 0, 0 0.023 (1) Å ²
No. of reflections	312	320	308	308
No. of profile points used	4088	4088	3936	3938
No. of Variables	81	47	89	92
R-factors ^a				
R _{wp}	0.1077	0.1678	0.1377	0.1318
R _p	0.0755	0.1131	0.1039	0.0915