

Structural, compositional and functional properties of Sb-doped Mg₂Si synthesized in Al₂O₃ - crucibles

Supplementary information

Structural and compositional characterization

Results of the fitting via Rietveld refinement of XRD Patterns for as-synthesized ingots

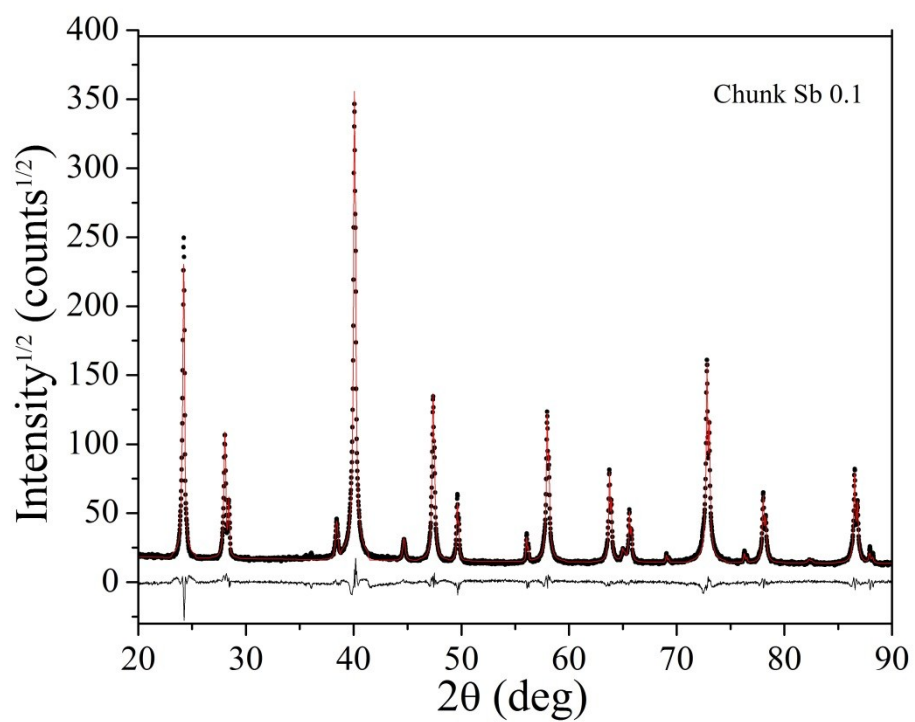
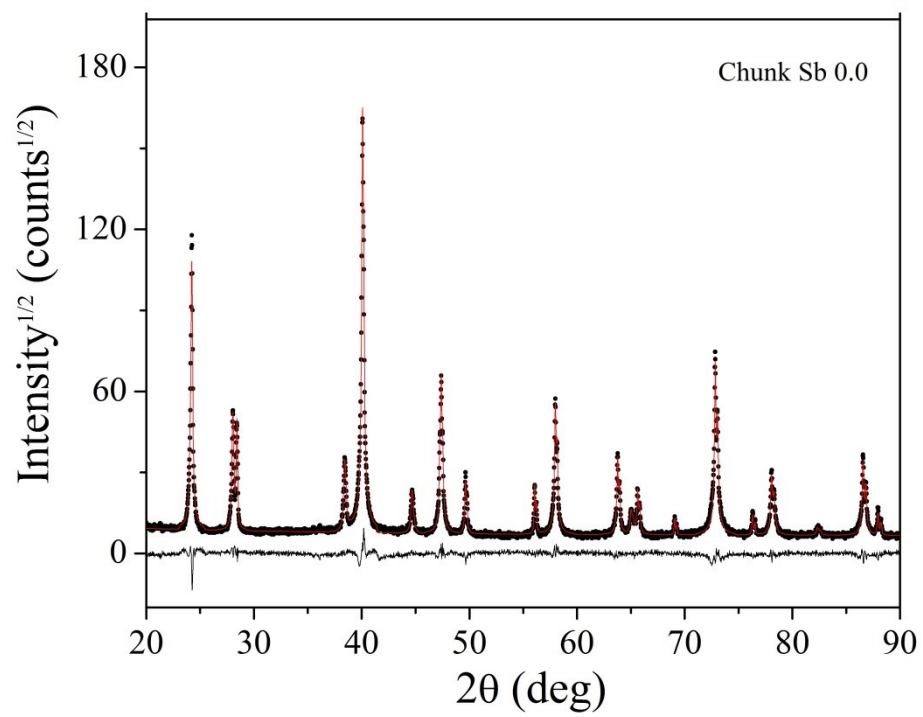
nominal Sb (at%)	phase content (wt %)		
	Mg ₂ Si	Si	Al
0	89.6±9.7	5.0±0.2	5.4±0.1
0.1	96.1±10.0	1.8±0.1	2.1±0.1
0.3	92.7±2.5	3.6±0.1	3.7±0.2
0.5	97.9±4.6	0.7±0.1	1.4±0.1
0.7	96.3±4.8	1.7±0.1	2.0±0.2
1	98.1±9.3	0.8±0.1	1.1±0.1
1.5	94.4±10.0	2.3±0.2	3.3±0.2

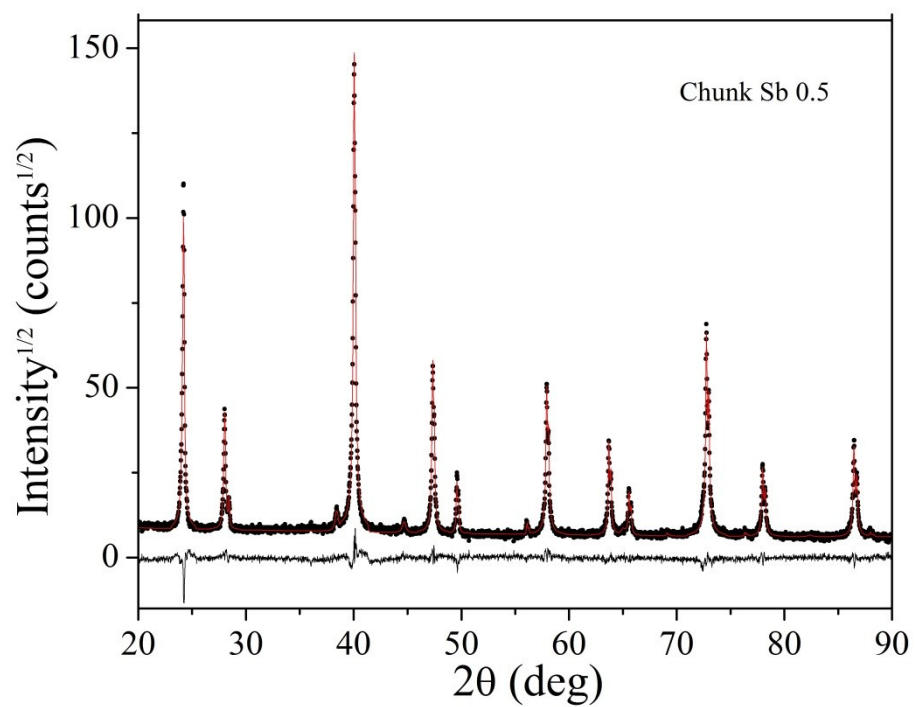
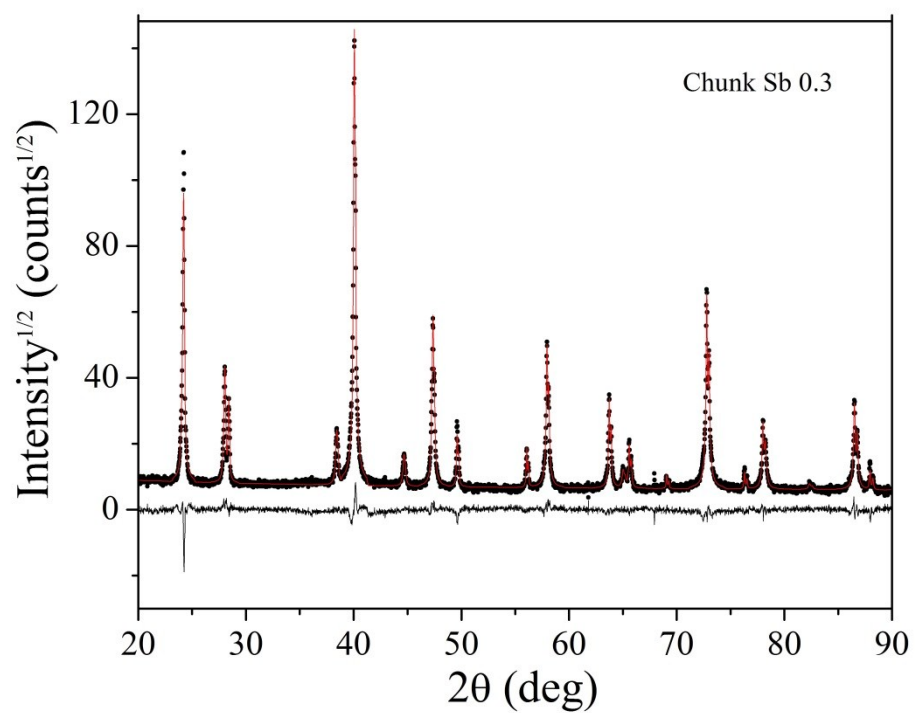
Rietveld refinement final R values for XRD patterns of as-synthesized ingots

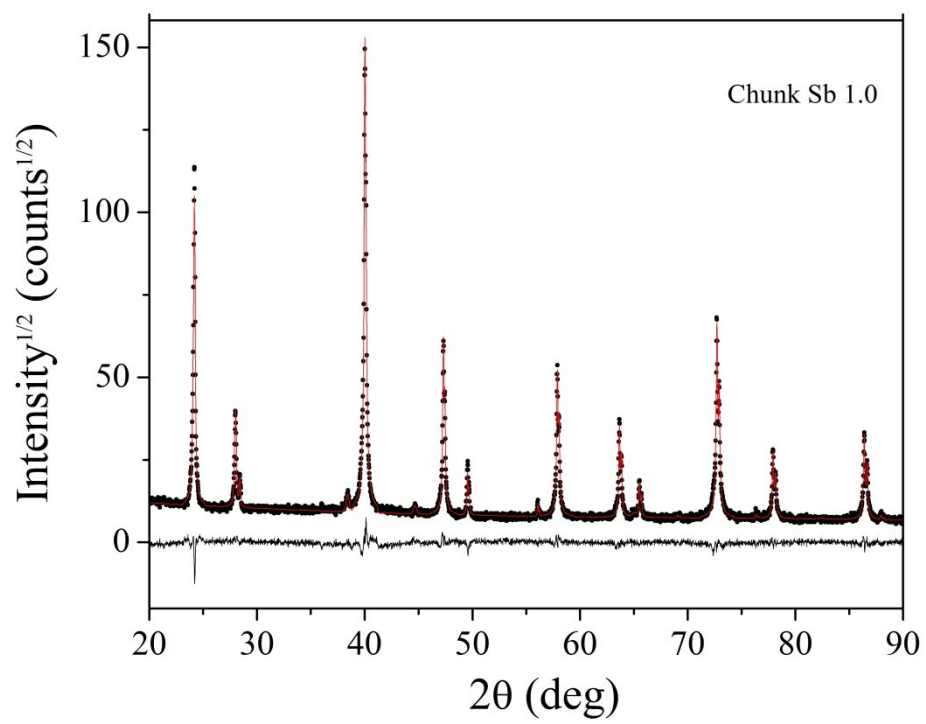
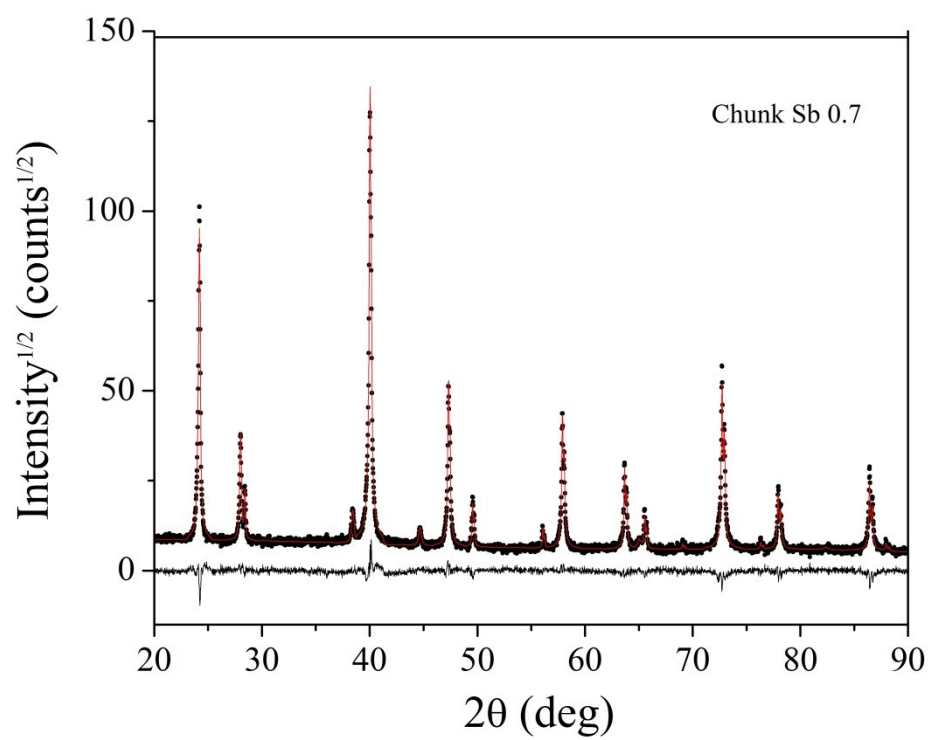
	Sb 0.0	Sb 0.1	Sb 0.3	Sb 0.5	Sb 0.7	Sb 1.0	Sb 1.5
R_{exp} (%)	6.64	3.21	7.05	6.89	7.68	6.65	2.58
R_{wp} (%)	12.49	10.27	14.12	12.78	13.04	11.31	9.44
R_b (%)	9.49	7.64	10.63	9.90	10.49	8.64	7.46
G.O.F.	1.88	3.20	2.00	1.86	1.70	1.70	3.70

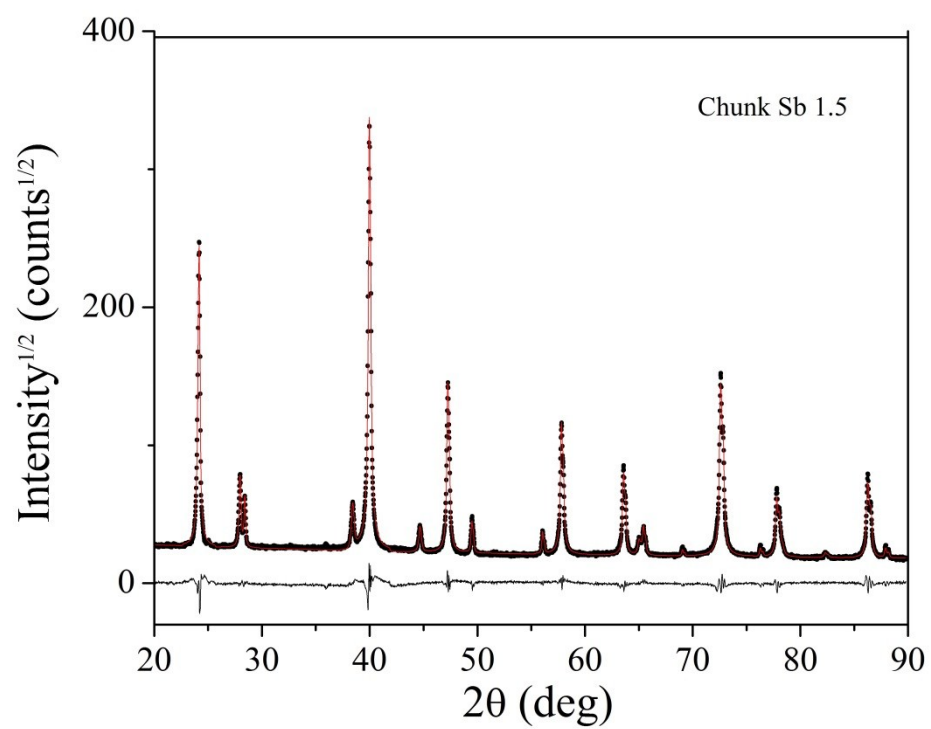
Metallic Al originated from the reaction between Mg and the Al₂O₃ crucibles used in synthesis step. MgO underwent surface segregation and it was possible to cut it off the ingots (MgO is detrimental for thermoelectric properties). For this reason it was not detected by means of XRD.

Observed (black dotted), and calculated (red line) XRD profiles and difference plots for as synthesized ingots









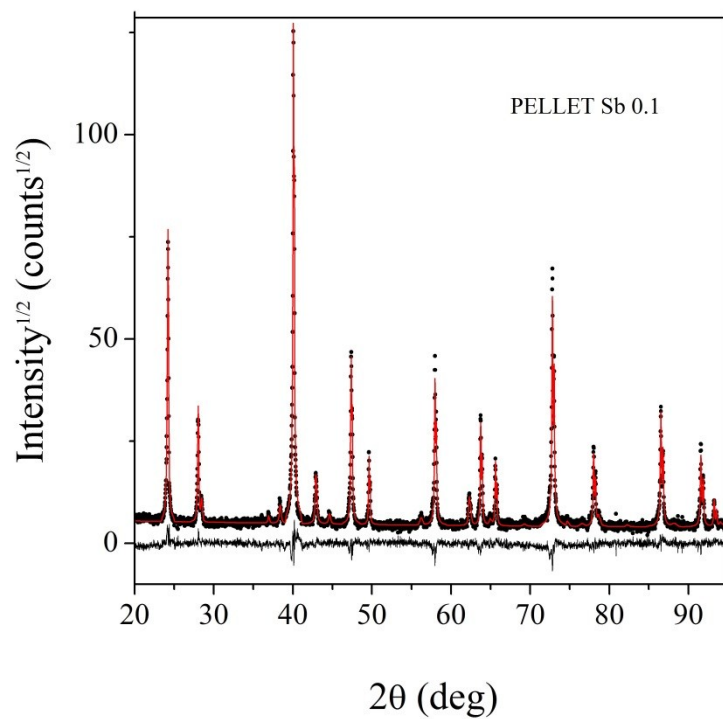
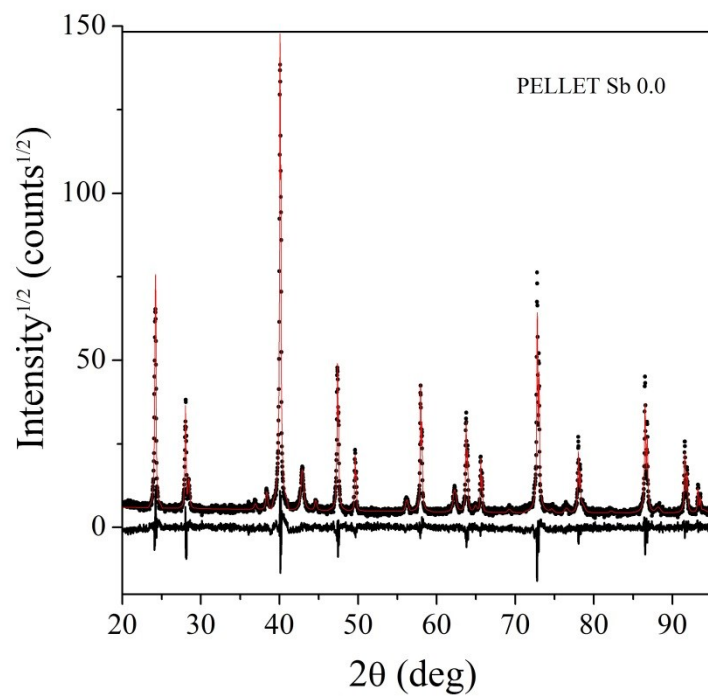
Results of the fitting via Rietveld refinement of XRD Patterns for sintered pellets

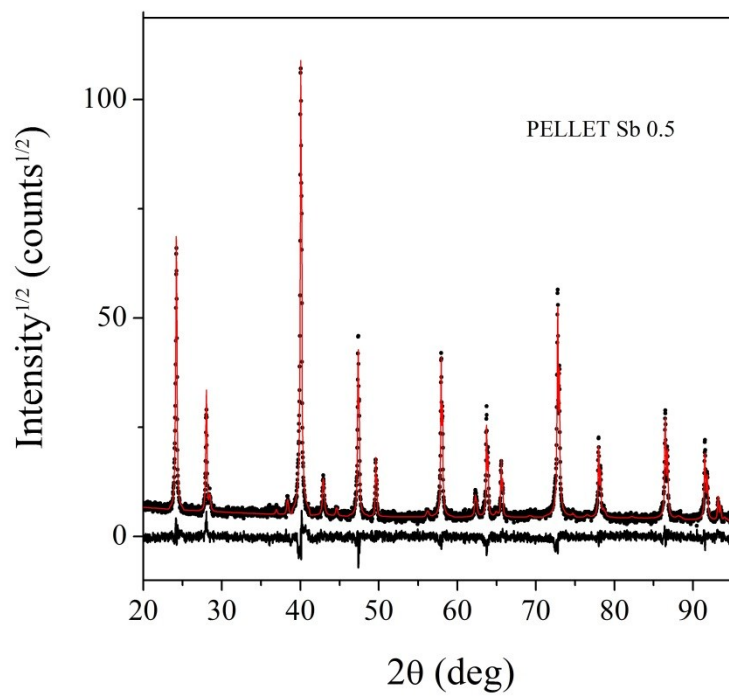
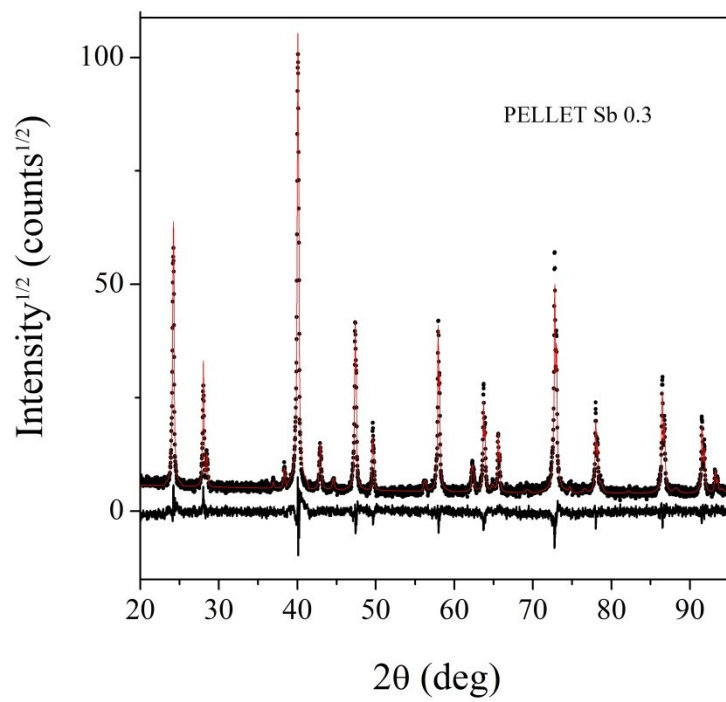
nominal Sb (at%)	phase content (wt %)		molar ratio
	Mg ₂ Si	MgO	MgO/Si
0	90.7±4.7	6.5±0.4	2.7
0.1	94.6±7.6	3.7±0.2	3.2
0.3	94.3±5.1	3.5±0.2	2.0
0.5	95.4±7.4	3.0±0.2	2.7
0.7	94.8±3.8	3.6±0.2	2.3
1	94.9±9.3	3.5±0.2	2.3
1.5	95.6±10.0	3.5±0.2	6.1

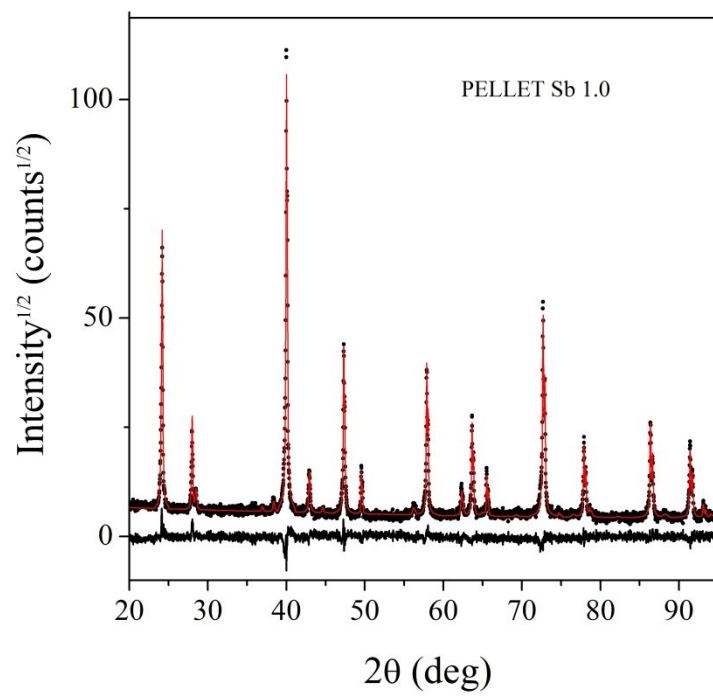
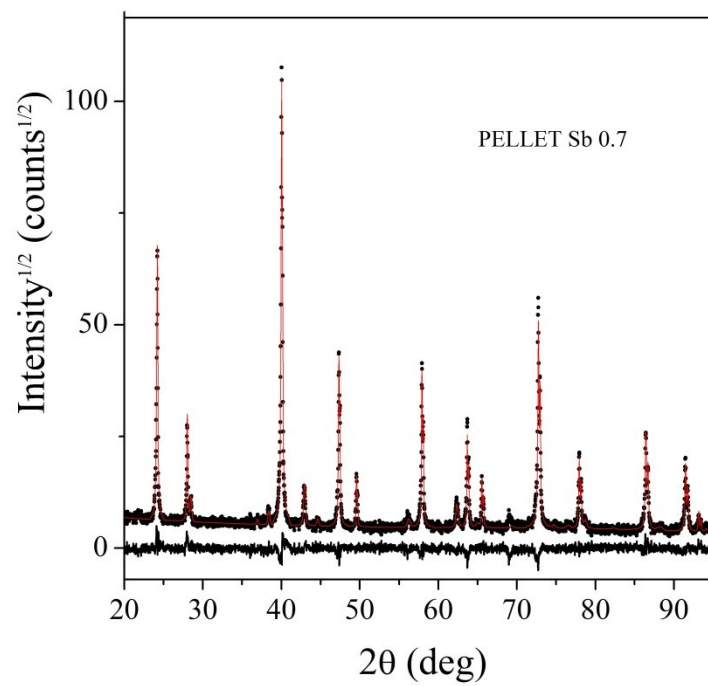
Rietveld refinement final R values for XRD patterns of sintered pellets

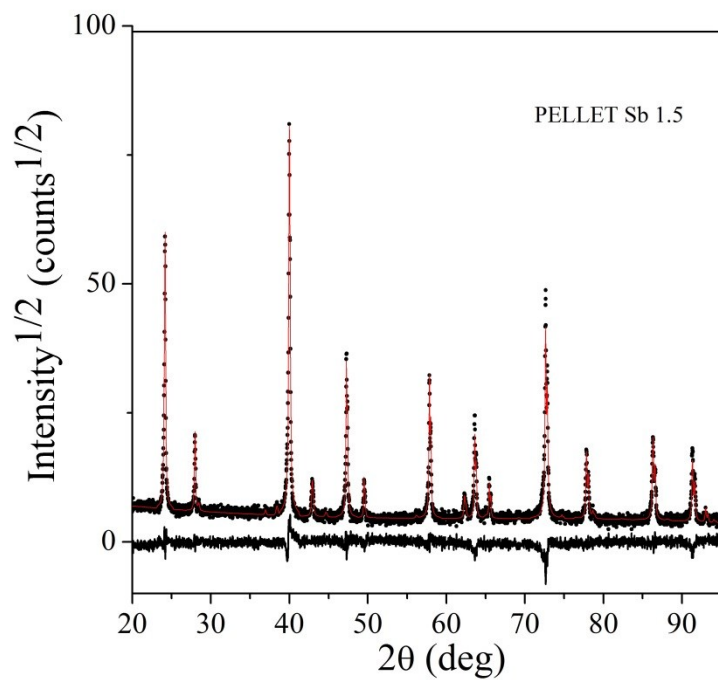
	Sb 0.0	Sb 0.1	Sb 0.3	Sb 0.5	Sb 0.7	Sb 1.0	Sb 1.5
R_{exp} (%)	8.61	9.57	10.04	10.20	10.46	10.31	11.76
R_{wp} (%)	20.02	16.00	18.00	16.03	15.65	15.28	18.47
R_b (%)	15.82	11.78	14.18	12.19	11.46	11.15	15.65
G.O.F.	2.32	1.67	1.80	1.57	1.50	1.48	1.63

Observed (black dotted) and calculated (red line) XRD profiles and difference plots for sintered pellets

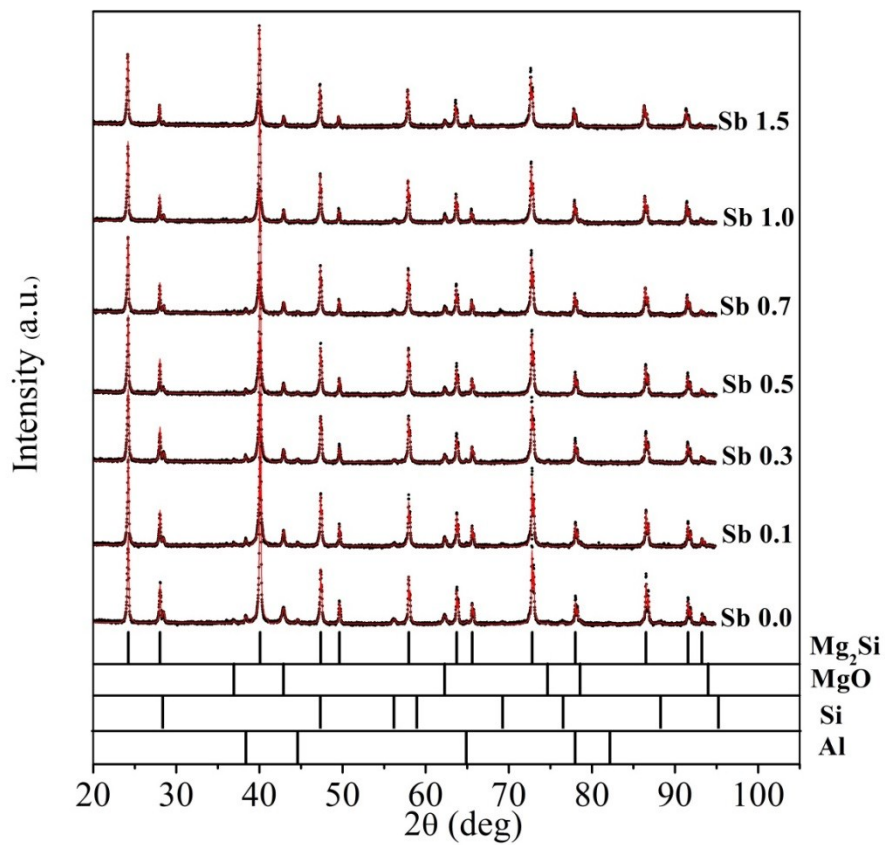








Superimposed XRD patterns (observed :black dotted; calculated: red line) of all sintered pellets



Density of sintered pellets

nominal Sb (at%)	theroetical (g/cm ³)	geometrical (g/cm ³)	relative (%)
0	2.049	2.003	97.8
0.1	2.029	2.008	99.0
0.3	2.046	2.019	98.7
0.5	2.049	2.022	98.7
0.7	2.074	2.026	97.7
1.0	2.083	2.060	98.9
1.5	2.147	2.088	97.2

Functional characterization

Lattice thermal conductivity calculated with lambda=0 and lamda=1 as a function of the dopant concentration.

