Electronic Supplementary Material (ESI) for Materials Advances.

Synergistic manifestation of band and scattering engineering in aliovalent alloyed anharmonic SnTe alloy

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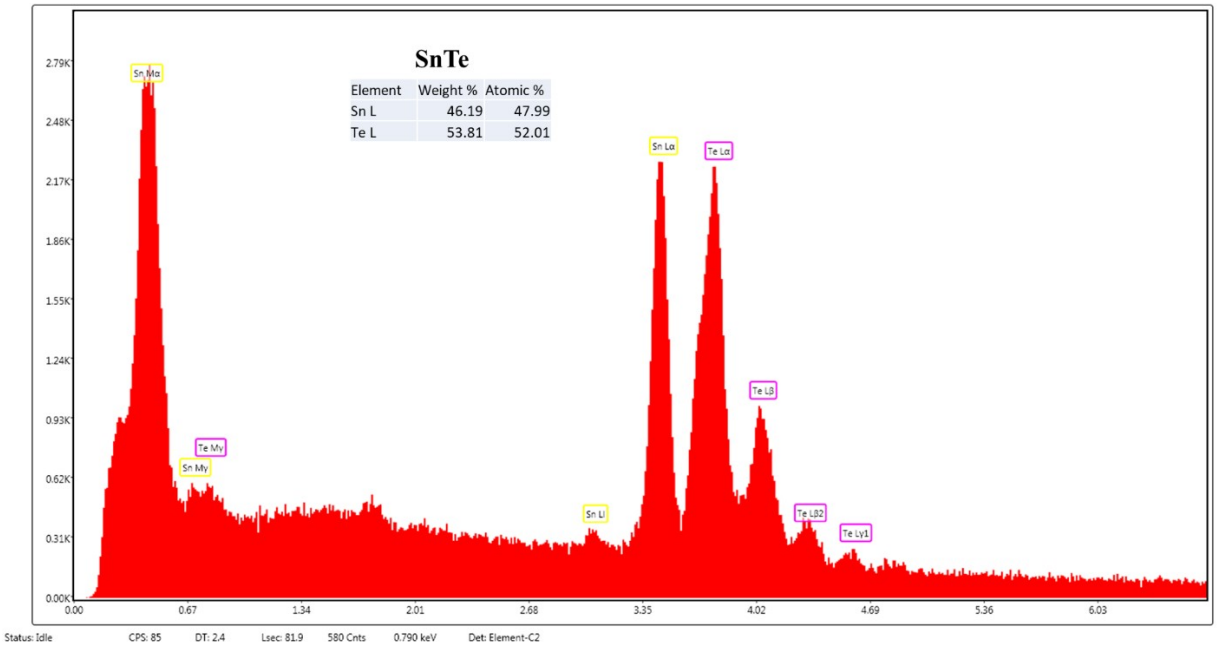
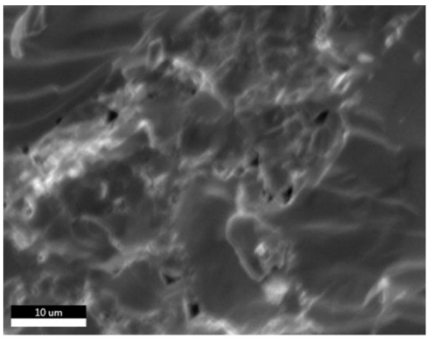
Supplementary Information

S1: EDS spectra and corresponding quantitative analysis as well as point scan of the nano-precipitates of Sb alloyed SnTe samples



SnTe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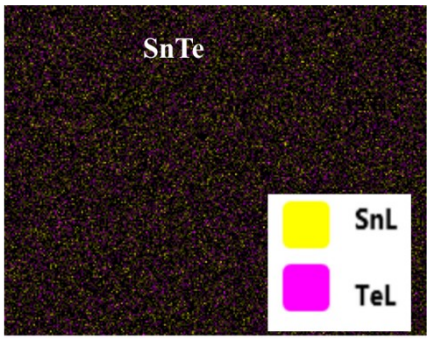
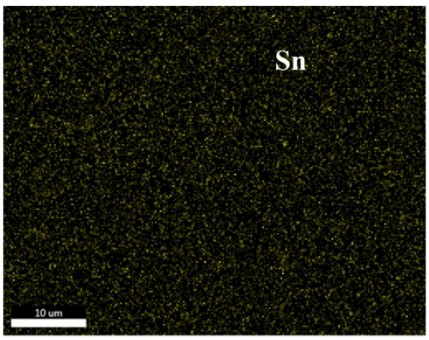

SnTe
SnL
TeL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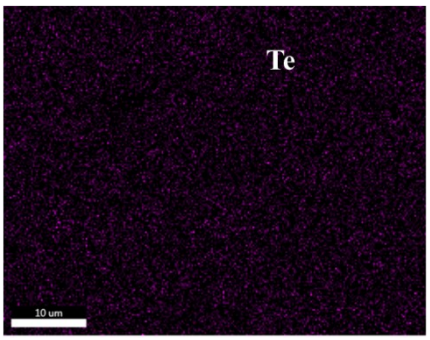
Te
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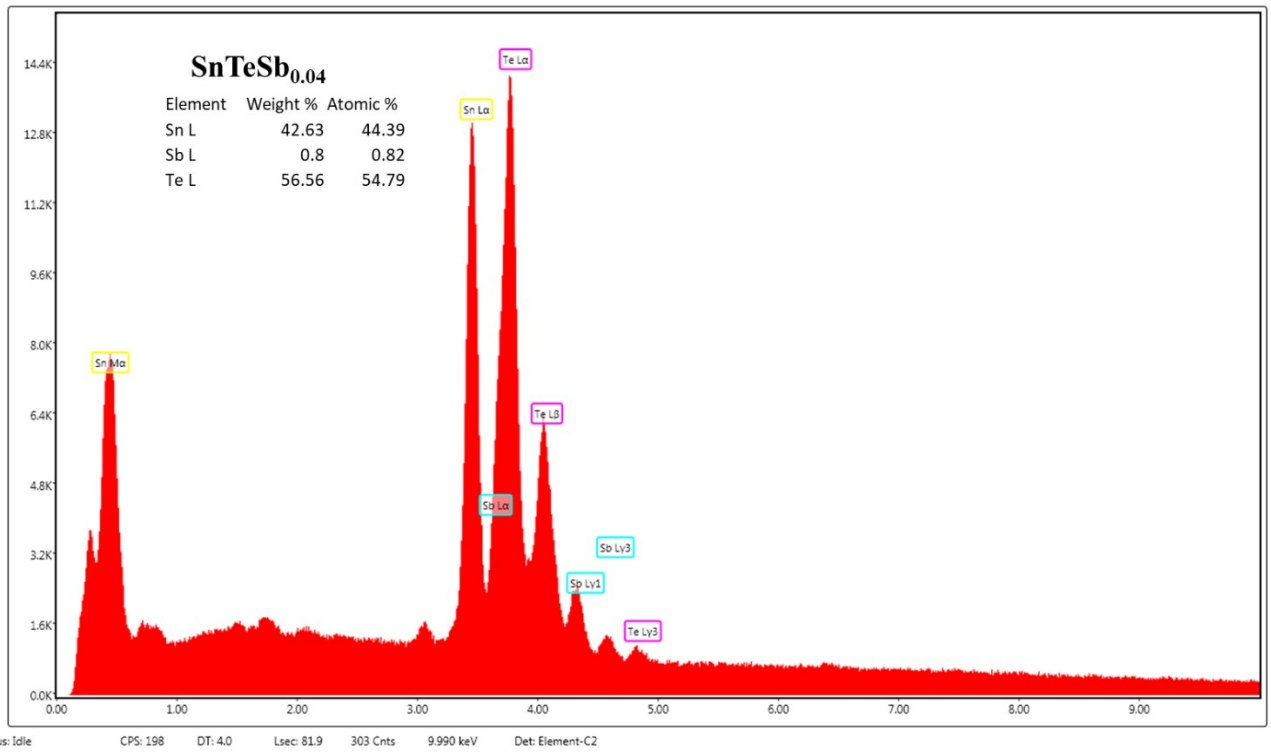
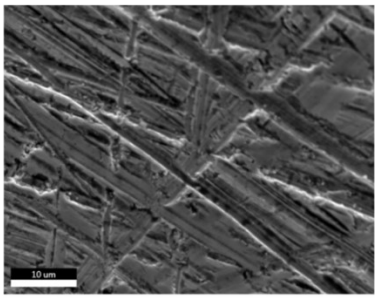

SnTeSb0.04
Element Weight % Atomic %
Sn L 42.63 44.39
Sb L 0.8 0.82
Te L 56.56 54.79
Te La
Sn La
Te Lß
Sb La
Sb Ly3
Sp Ly1
Te Ly3
Sn Mα
14.4K
12.8K
11.2K
9.6K
8.0K
6.4K
4.8K
3.2K
1.6K
0.0K
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
9.00
Status: Idle
CPS: 198
DT: 4.0
Lsec: 81.9
303 Cnts
9.990 keV
Det: Element-C2

$SnTeSb_{0.04}$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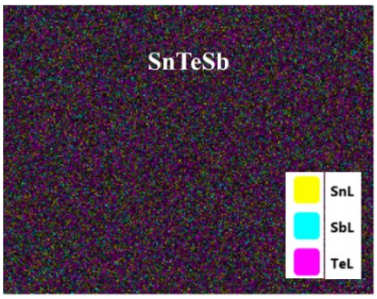
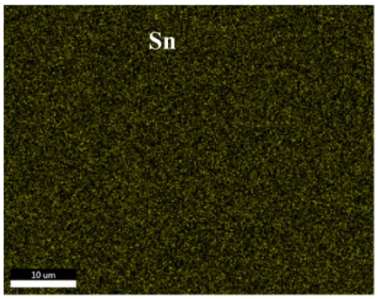

SnTeSb
SnL
SbL
TeL


Sn
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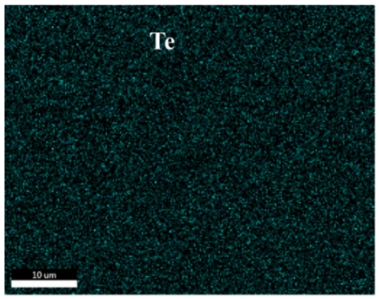
Te
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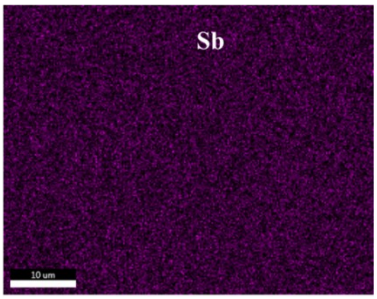
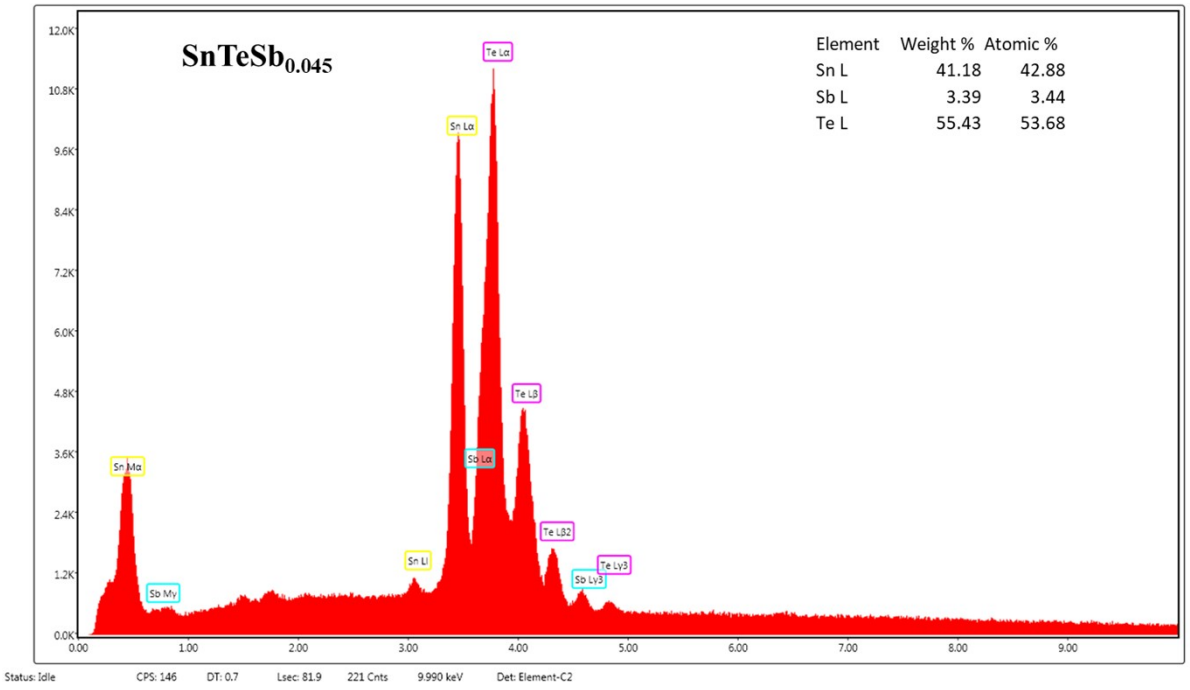
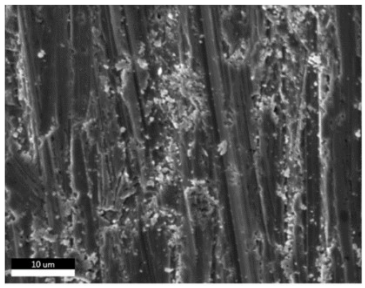
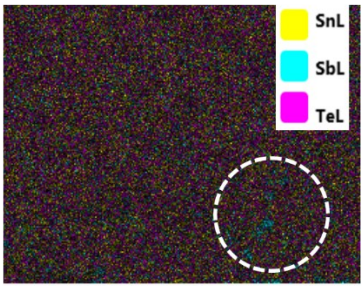
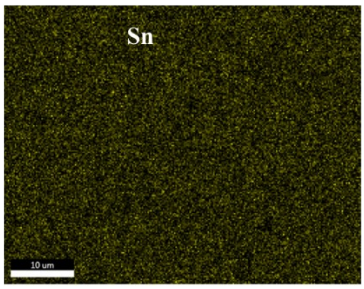

Sb
10 um

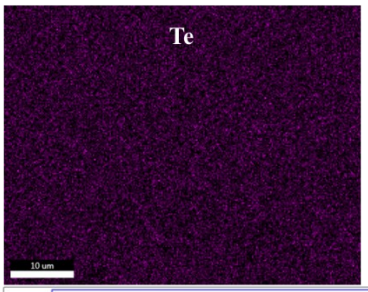

SnTeSb0.045
Element Weight % Atomic %
Sn L 41.18 42.88
Sb L 3.39 3.44
Te L 55.43 53.68
Te Lα
Sn Lα
Te Lβ
Sb Lα
Te Lβ2
Te Lγ3
Sb Lγ3
Sn Ma
Sb Mγ
Sn Li
12.0K
10.8K
9.6K
8.4K
7.2K
6.0K
4.8K
3.6K
2.4K
1.2K
0.0K
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
9.00
Status: Idle
CPS: 146
DT: 0.7
Lsec: 81.9
221 Cnts
9.990 keV
Det: Element-C2

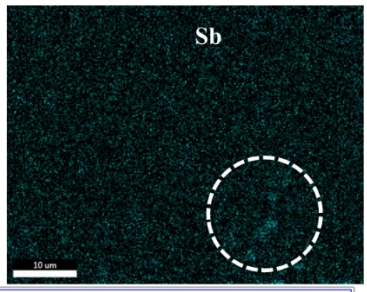
$SnTeSb_{0.045}$



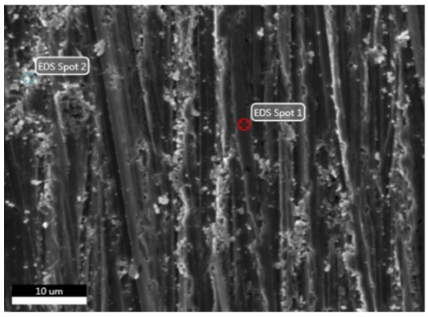


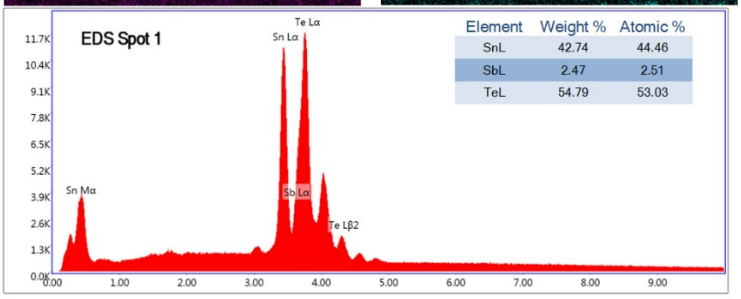




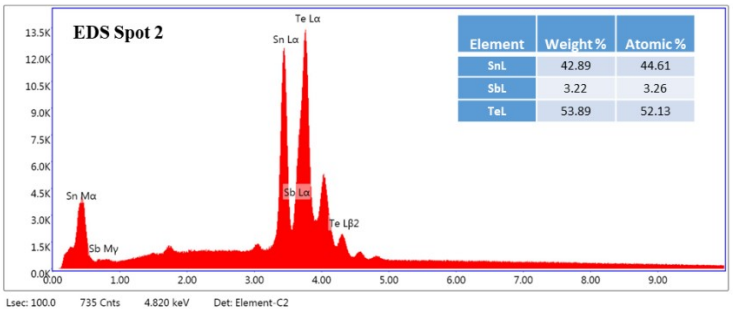


$SnTeSb_{0.045}$

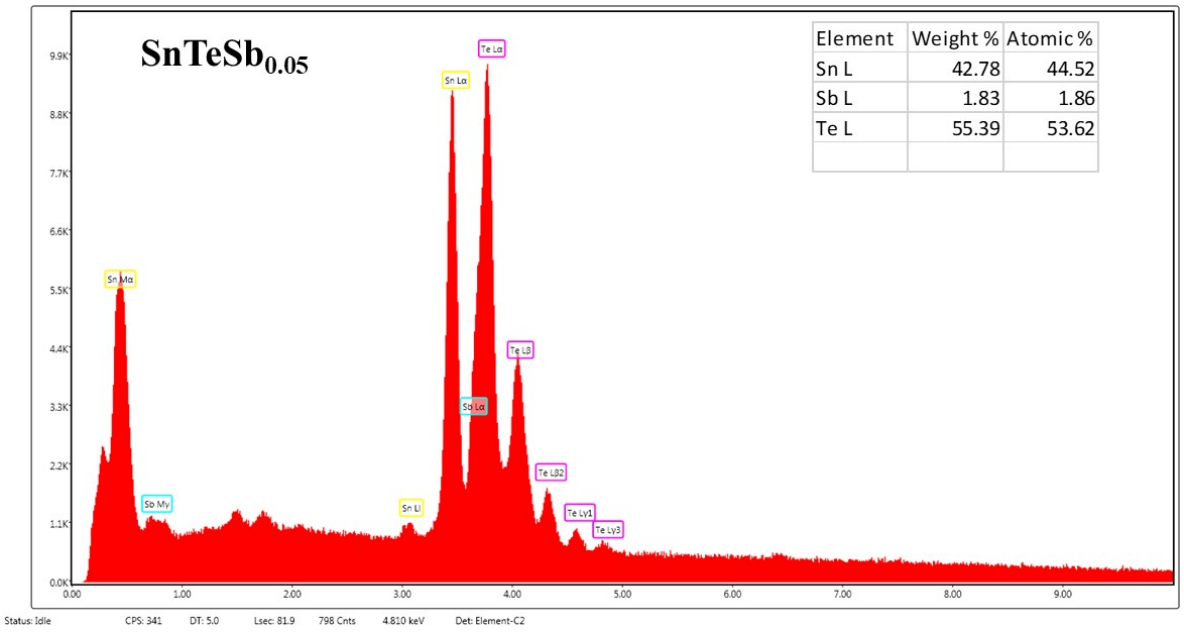




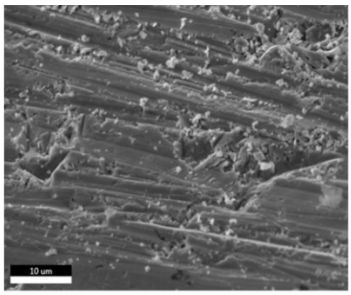
Element	Weight %	Atomic %
SnL	42.74	44.46
SbL	2.47	2.51
TeL	54.79	53.03



Element	Weight %	Atomic %
SnL	42.89	44.61
SbL	3.22	3.26
TeL	53.89	52.13


SnTeSb0.05
Element | Weight % | Atomic %
Sn L | 42.78 | 44.52
Sb L | 1.83 | 1.86
Te L | 55.39 | 53.62
Sn Mα
Sb Mγ
Sn Lℓ
Sn Lα
Sb Lα
Te Lα
Te Lβ
Te Lβ2
Te Lγ1
Te Lγ3
0.0K
1.1K
2.2K
3.3K
4.4K
5.5K
6.6K
7.7K
8.8K
9.9K
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
9.00
Status: Idle
CPS: 341
DT: 5.0
Lsec: 81.9
798 Cnts
4.810 keV
Det: Element-C2

$SnTeSb_{0.05}$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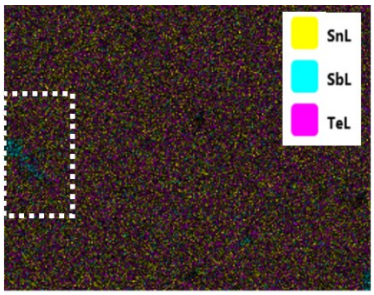
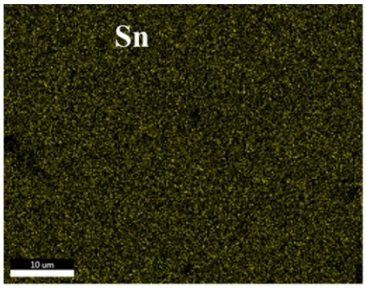

SnL
SbL
TeL


Sn
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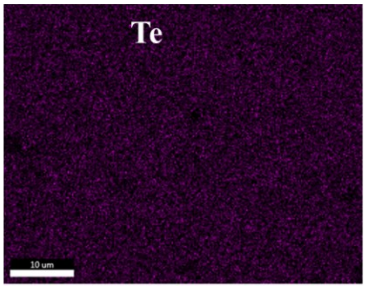
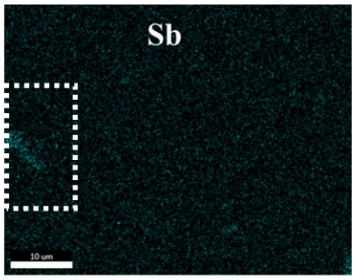
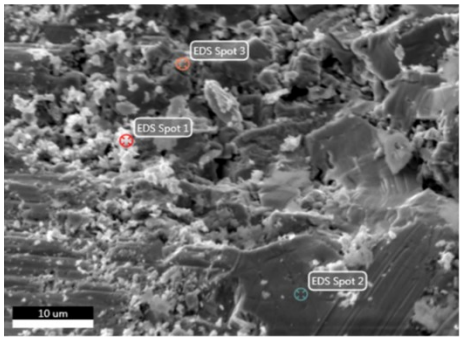
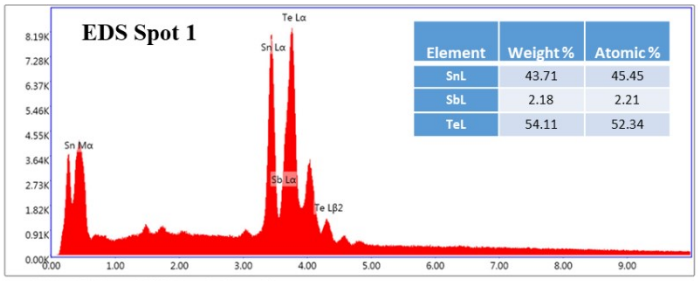
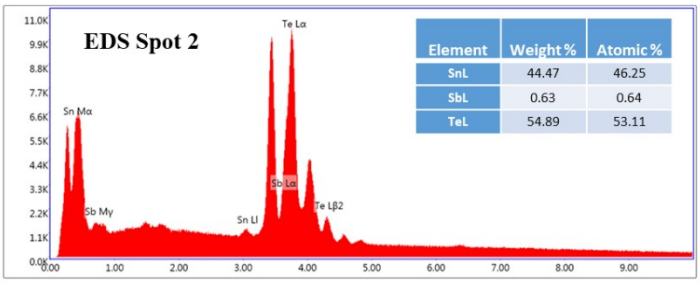

Te
10 um

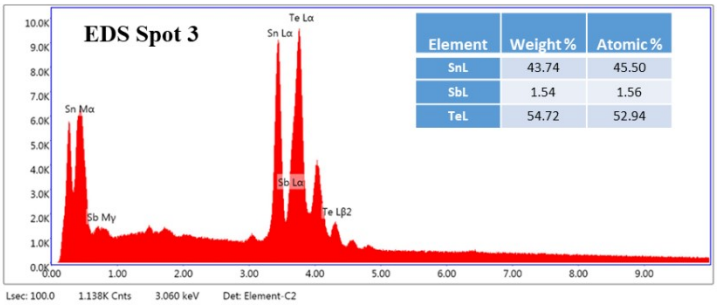

Sb
10 um

$SnTeSb_{0.05}$





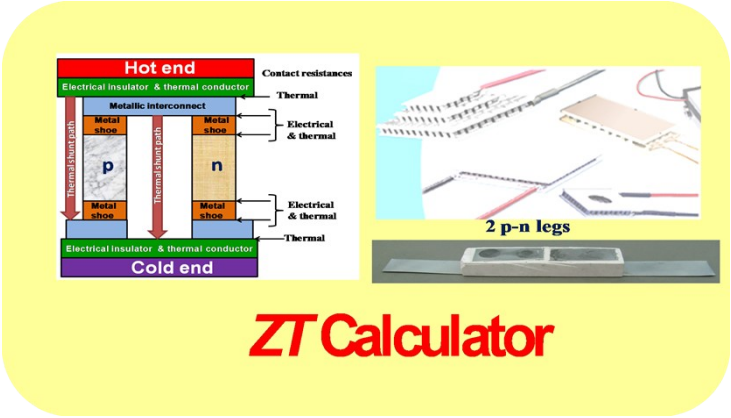




S2: Calculation of *L* value obtained from the accepted methodology of fitting the Seebeck data to the reduced chemical potential

Temperature (K)	Seebeck (μV/K)	Fitted Seebeck (μV/K)	η,reduced chemical potential	orenz Number ($x10^{-8}$ $W\Omega K^{-2}$	Hall Factor, r_H	Hall coefficient, $[m^3c^{-1}]$	carrier density, m^{-3}	m^*/m_o
300	112.831	112.7351572	1.994522171	1.863855941	1.09067327 6	8.93E-002	7.63E+19	0.00011
322.47047	325.576	325.5872732	-1.688974342	1.528552868	1.185797834	1.30E-007	5.70E+25	5.82932
366.66394	346.8913	346.9032137	-1.955286413	1.521773419	1.188405998	1.30E-007	5.71E+25	6.08591
414.4298	371.4039	371.4062539	-2.256121525	1.515795257	1.190734873	1.30E-007	5.72E+25	6.54605
462.6243	387.3152	387.344994	-2.449446972	1.512725878	1.191941258	1.30E-007	5.73E+25	6.65317
510.557	408.2097	408.2554686	-2.70087223	1.509470677	1.19322865	1.30E-007	5.74E+25	7.10893
558.6706	423.9881	424.0031153	-2.888881715	1.507490789	1.194015708	1.30E-007	5.74E+25	7.35192
606.8872	429.8385	429.8596024	-2.958554508	1.50684195	1.194274305	1.30E-007	5.74E+25	7.08572
655.1944	450.3333	450.2891239	-3.20070889	1.50489434	1.195052515	1.30E-007	5.75E+25	7.70059
703.3427	461.5267	461.4759486	-3.332802384	1.504007923	1.19540769	1.30E-007	5.75E+25	7.82801

S3: Calculation of maximum efficiency



Although there is no analytic expression for Z, it can be calculated to any desired accuracy numerically with a simple procedure which can be done on a spreadsheet. To calculate the maximum efficiency Z and ZT follow these steps:

(1) Paste the temperature dependent $S(T)$, $\rho(T)$, and $\kappa(T)$into the T, S, ρ, and κ columns – the 4 columns in the table are shaded blue. The cold side temperature for the calculation is the first temperature, 300 K. We shall use 800 K for hot side temperature for the example in Table 1. As per the literature, 25 K temperature intervals were maintained between data points, but that can vary. Smaller temperature steps give more accurate calculations.

(2) The first entry of the relative current value u is to be optimized. The values for u at higher temperature will adjust accordingly. This is similar to setting the electrical current (or load resistance) through the device. The power and therefore efficiency will be low at low values of u because little electrical current will be flowing through the device and low at high values of u because the output voltage will drop at high currents (and even becomes negative). For good efficiency the u values should be close to the compatibility factor s in the column next to u. Calculation for u = 0 is to be avoided as some calculations become undefined, but u arbitrarily small is fine (e.g. u = 0.001).

The efficiency of this thermoelectric leg is given in the efficiency column. The calculation assumes the first row (300 K in the Table) is the cold side. For 800 K hot side we should optimize the efficiency of the last row. MS Excel has a solver add-in that makes this easy,but other methods or adjusting by hand also works.

(3) The device ZT is calculated from the maximum efficiency value found by optimizing cold side u value and the eqn. is given by $ZT = \left(\frac{T_h - T_c(1-\eta)}{T_h(1-\eta) - T_c}\right)^2 - 1$.

S.3.1 Spreadsheet for the calculation of ZT for SnTe

T (C)	Material	T (K)	Seebeck (μV/K)	resistivity (10-3 Ω cm)	thermal cond (W/m K)	zT	max red eff	s (1/V)	u (1/V)	red eff	Φ (V)	efficiency	ZT
27	p-SnTe	300	34	0.13	7.35	0.04	0.9%	1.76	1.6573	0.9%	0.614		
52	p-SnTe	325	35	0.14	7.16	0.04	1.0%	1.73	1.6595	1.0%	0.614	0.1%	0.04
77	p-SnTe	350	36	0.15	6.97	0.04	1.1%	1.70	1.6619	1.1%	0.614	0.1%	0.04
102	p-SnTe	375	38	0.16	6.78	0.05	1.2%	1.67	1.6646	1.2%	0.615	0.2%	0.04
127	p-SnTe	400	39	0.18	6.59	0.05	1.3%	1.64	1.6675	1.3%	0.615	0.3%	0.04
152	p-SnTe	425	41	0.19	6.41	0.06	1.4%	1.62	1.6707	1.4%	0.616	0.4%	0.05
177	p-SnTe	450	42	0.21	6.23	0.06	1.5%	1.60	1.6743	1.5%	0.616	0.5%	0.05
202	p-SnTe	475	44	0.23	6.04	0.07	1.6%	1.59	1.6783	1.6%	0.617	0.6%	0.05
227	p-SnTe	500	46	0.25	5.86	0.07	1.8%	1.58	1.6827	1.8%	0.617	0.6%	0.05
252	p-SnTe	525	49	0.26	5.68	0.08	2.0%	1.58	1.6877	2.0%	0.618	0.7%	0.06
277	p-SnTe	550	51	0.28	5.51	0.09	2.2%	1.59	1.6933	2.2%	0.619	0.8%	0.06
302	p-SnTe	575	54	0.31	5.33	0.10	2.4%	1.61	1.6996	2.4%	0.619	0.9%	0.06
327	p-SnTe	600	57	0.33	5.15	0.11	2.7%	1.63	1.7067	2.7%	0.620	1.0%	0.06
352	p-SnTe	625	60	0.35	4.98	0.13	3.0%	1.66	1.7146	3.0%	0.621	1.1%	0.07
377	p-SnTe	650	63	0.37	4.80	0.14	3.4%	1.70	1.7234	3.4%	0.621	1.3%	0.07
402	p-SnTe	675	67	0.40	4.63	0.16	3.8%	1.75	1.7334	3.8%	0.622	1.4%	0.08
427	p-SnTe	700	71	0.43	4.45	0.19	4.3%	1.80	1.7445	4.3%	0.623	1.6%	0.08
452	p-SnTe	725	76	0.45	4.28	0.22	4.9%	1.86	1.7570	4.9%	0.624	1.7%	0.09
477	p-SnTe	750	81	0.48	4.10	0.25	5.5%	1.93	1.7710	5.5%	0.625	1.9%	0.09
502	p-SnTe	775	86	0.51	3.93	0.29	6.3%	2.00	1.7867	6.2%	0.626	2.1%	0.10

S.3.2 Spreadsheet for the calculation of ZT for $SnTeSb_{0.02}$

T	Material	*T*	Seebeck	resistivity	thermal cond	*zT*	max red eff	*s*	*u*	red eff	Φ	efficiency	*ZT*
(C)		(K)	(μV/K)	(10-3 Ω cm)	(W/m K)			(1/V)	(1/V)		(V)		
27	p-SnTeSb_0.02	300	29	0.16	7.05	0.02	0.6%	1.30	1.8532	0.5%	0.548		
52	p-SnTeSb_0.02	325	30	0.17	6.85	0.02	0.6%	1.29	1.8558	0.5%	0.548	0.0%	0.02
77	p-SnTeSb_0.02	350	31	0.18	6.66	0.03	0.7%	1.32	1.8598	0.6%	0.549	0.1%	0.02
102	p-SnTeSb_0.02	375	33	0.19	6.48	0.03	0.8%	1.36	1.8644	0.7%	0.549	0.1%	0.02
127	p-SnTeSb_0.02	400	36	0.20	6.29	0.04	1.0%	1.41	1.8698	0.9%	0.549	0.2%	0.03
152	p-SnTeSb_0.02	425	39	0.22	6.10	0.05	1.2%	1.46	1.8760	1.1%	0.550	0.2%	0.03
177	p-SnTeSb_0.02	450	42	0.23	5.89	0.06	1.4%	1.53	1.8832	1.4%	0.550	0.3%	0.03
202	p-SnTeSb_0.02	475	46	0.25	5.69	0.07	1.7%	1.60	1.8914	1.7%	0.550	0.4%	0.04
227	p-SnTeSb_0.02	500	50	0.26	5.49	0.09	2.1%	1.69	1.9015	2.0%	0.551	0.5%	0.04
252	p-SnTeSb_0.02	525	53	0.28	5.29	0.10	2.4%	1.75	1.9103	2.4%	0.551	0.6%	0.04
277	p-SnTeSb_0.02	550	58	0.30	5.09	0.12	2.8%	1.83	1.9221	2.8%	0.552	0.7%	0.05
302	p-SnTeSb_0.02	575	63	0.32	4.88	0.15	3.4%	1.94	1.9364	3.4%	0.553	0.8%	0.06
327	p-SnTeSb_0.02	600	68	0.35	4.67	0.17	4.0%	2.02	1.9502	4.0%	0.554	1.0%	0.06
352	p-SnTeSb_0.02	625	74	0.37	4.45	0.20	4.6%	2.12	1.9656	4.6%	0.555	1.2%	0.07
377	p-SnTeSb_0.02	650	80	0.40	4.24	0.24	5.4%	2.22	1.9840	5.4%	0.556	1.4%	0.08
402	p-SnTeSb_0.02	675	85	0.44	4.03	0.28	6.1%	2.28	2.0019	6.1%	0.557	1.6%	0.09
427	p-SnTeSb_0.02	700	91	0.46	3.81	0.33	7.1%	2.39	2.0218	6.9%	0.558	1.8%	0.10
452	p-SnTeSb_0.02	725	97	0.50	3.60	0.38	8.1%	2.50	2.0439	7.9%	0.560	2.1%	0.11
477	p-SnTeSb_0.02	750	104	0.54	3.38	0.44	9.1%	2.57	2.0683	8.8%	0.561	2.4%	0.12
502	p-SnTeSb_0.02	775	111	0.58	3.16	0.52	10.5%	2.72	2.0954	10.0%	0.563	2.7%	0.13

S.3.3 Spreadsheet for the calculation of ZT for $SnTeSb_{0.03}$

T	Material	*T*	Seebeck	resistivity	thermal cond	*zT*	max red eff	*s*	*u*	red eff	Φ	efficiency	*ZT*
(C)		(K)	(μV/K)	(10-3 Ω cm)	(W/m K)			(1/V)	(1/V)		(V)		
27	p-SnTeSb_0.03	300	24	0.19	6.10	0.02	0.4%	1.04	1.9430	0.1%	0.522		
52	p-SnTeSb_0.03	325	26	0.20	5.87	0.02	0.5%	1.10	1.9473	0.2%	0.522	0.0%	0.01
77	p-SnTeSb_0.03	350	29	0.21	5.66	0.02	0.6%	1.17	1.9525	0.3%	0.522	0.0%	0.01
102	p-SnTeSb_0.03	375	31	0.23	5.45	0.03	0.7%	1.23	1.9579	0.5%	0.522	0.1%	0.01
127	p-SnTeSb_0.03	400	34	0.24	5.25	0.04	0.9%	1.33	1.9649	0.7%	0.522	0.1%	0.01
152	p-SnTeSb_0.03	425	37	0.26	5.05	0.05	1.1%	1.43	1.9730	1.0%	0.523	0.1%	0.02
177	p-SnTeSb_0.03	450	41	0.27	4.83	0.06	1.4%	1.54	1.9822	1.3%	0.523	0.2%	0.02
202	p-SnTeSb_0.03	475	45	0.29	4.63	0.07	1.7%	1.64	1.9919	1.6%	0.523	0.3%	0.03
227	p-SnTeSb_0.03	500	49	0.31	4.44	0.09	2.1%	1.74	2.0029	2.1%	0.524	0.4%	0.03
252	p-SnTeSb_0.03	525	55	0.34	4.25	0.11	2.6%	1.86	2.0163	2.6%	0.525	0.5%	0.04
277	p-SnTeSb_0.03	550	60	0.36	4.06	0.13	3.1%	1.96	2.0302	3.1%	0.525	0.6%	0.04
302	p-SnTeSb_0.03	575	65	0.39	3.88	0.16	3.8%	2.09	2.0472	3.8%	0.526	0.8%	0.05
327	p-SnTeSb_0.03	600	72	0.42	3.69	0.20	4.5%	2.21	2.0661	4.5%	0.527	1.0%	0.06
352	p-SnTeSb_0.03	625	79	0.45	3.51	0.24	5.5%	2.35	2.0885	5.4%	0.528	1.2%	0.07
377	p-SnTeSb_0.03	650	86	0.49	3.34	0.30	6.5%	2.47	2.1135	6.4%	0.529	1.4%	0.08
402	p-SnTeSb_0.03	675	94	0.53	3.17	0.35	7.5%	2.58	2.1398	7.4%	0.531	1.6%	0.09
427	p-SnTeSb_0.03	700	101	0.58	3.01	0.41	8.6%	2.67	2.1676	8.4%	0.532	1.9%	0.10
452	p-SnTeSb_0.03	725	109	0.63	2.85	0.48	9.8%	2.75	2.1985	9.5%	0.534	2.2%	0.11
477	p-SnTeSb_0.03	750	117	0.68	2.69	0.56	11.1%	2.84	2.2330	10.7%	0.536	2.6%	0.13
502	p-SnTeSb_0.03	775	126	0.74	2.54	0.65	12.4%	2.92	2.2713	11.9%	0.538	2.9%	0.14

S.3.4 Spreadsheet for the calculation of ZT for $SnTeSb_{0.035}$

T	Material	*T*	Seebeck	resistivity	thermal cond	*zT*	max red eff	*s*	*u*	red eff	Φ	efficiency	*ZT*
(C)		(K)	(μV/K)	(10-3 Ω cm)	(W/m K)			(1/V)	(1/V)		(V)		
27	p-SnTeSb_0.035	300	20	0.17	6.60	0.01	0.3%	0.88	1.8676	-0.1%	0.541		
52	p-SnTeSb_0.035	325	23	0.18	6.36	0.01	0.4%	0.96	1.8721	0.0%	0.541	0.0%	0.00
77	p-SnTeSb_0.035	350	25	0.19	6.13	0.02	0.5%	1.04	1.8770	0.2%	0.542	0.0%	0.00
102	p-SnTeSb_0.035	375	28	0.21	5.90	0.02	0.6%	1.13	1.8826	0.3%	0.542	0.0%	0.00
127	p-SnTeSb_0.035	400	31	0.22	5.67	0.03	0.8%	1.22	1.8892	0.5%	0.542	0.1%	0.01
152	p-SnTeSb_0.035	425	35	0.24	5.45	0.04	1.0%	1.32	1.8967	0.8%	0.542	0.1%	0.01
177	p-SnTeSb_0.035	450	39	0.26	5.22	0.05	1.2%	1.43	1.9054	1.1%	0.542	0.1%	0.01
202	p-SnTeSb_0.035	475	43	0.28	4.99	0.06	1.6%	1.54	1.9153	1.5%	0.543	0.2%	0.02
227	p-SnTeSb_0.035	500	48	0.30	4.77	0.08	1.9%	1.66	1.9265	1.9%	0.543	0.3%	0.02
252	p-SnTeSb_0.035	525	53	0.32	4.55	0.10	2.4%	1.77	1.9391	2.4%	0.544	0.4%	0.03
277	p-SnTeSb_0.035	550	59	0.35	4.34	0.13	3.0%	1.88	1.9534	3.0%	0.544	0.5%	0.04
302	p-SnTeSb_0.035	575	65	0.38	4.13	0.16	3.6%	2.00	1.9694	3.6%	0.545	0.7%	0.04
327	p-SnTeSb_0.035	600	71	0.41	3.91	0.19	4.3%	2.12	1.9873	4.3%	0.546	0.8%	0.05
352	p-SnTeSb_0.035	625	78	0.45	3.70	0.23	5.2%	2.24	2.0073	5.1%	0.547	1.0%	0.06
377	p-SnTeSb_0.035	650	86	0.49	3.50	0.28	6.1%	2.35	2.0296	6.0%	0.548	1.3%	0.07
402	p-SnTeSb_0.035	675	93	0.53	3.29	0.33	7.2%	2.46	2.0545	7.0%	0.550	1.5%	0.08
427	p-SnTeSb_0.035	700	101	0.58	3.10	0.40	8.4%	2.58	2.0821	8.1%	0.551	1.8%	0.09
452	p-SnTeSb_0.035	725	110	0.63	2.90	0.48	9.7%	2.70	2.1128	9.3%	0.553	2.1%	0.11
477	p-SnTeSb_0.035	750	119	0.69	2.70	0.57	11.2%	2.83	2.1470	10.6%	0.555	2.4%	0.12
502	p-SnTeSb_0.035	775	128	0.75	2.51	0.68	12.8%	2.97	2.1849	12.1%	0.557	2.8%	0.14

S.3.5 Spreadsheet for the calculation of ZT for $SnTeSb_{0.04}$

T	Material	*T*	Seebeck	resistivity	thermal cond	*zT*	max red eff	*s*	*u*	red eff	Φ	efficiency	*ZT*
(C)		(K)	(μV/K)	(10-3 Ω cm)	(W/m K)			(1/V)	(1/V)		(V)		
27	p-SnTeSb_0.04	300	20	0.20	6.27	0.01	0.2%	0.79	1.6835	-0.1%	0.600		
52	p-SnTeSb_0.04	325	23	0.22	6.06	0.01	0.3%	0.86	1.6871	0.0%	0.600	0.0%	0.00
77	p-SnTeSb_0.04	350	25	0.23	5.87	0.02	0.4%	0.92	1.6911	0.1%	0.600	0.0%	0.00
102	p-SnTeSb_0.04	375	28	0.25	5.67	0.02	0.5%	1.00	1.6957	0.3%	0.600	0.0%	0.00
127	p-SnTeSb_0.04	400	31	0.26	5.48	0.03	0.7%	1.08	1.7012	0.5%	0.600	0.0%	0.01
152	p-SnTeSb_0.04	425	35	0.28	5.28	0.04	0.9%	1.17	1.7074	0.7%	0.601	0.1%	0.01
177	p-SnTeSb_0.04	450	39	0.30	5.07	0.05	1.1%	1.27	1.7146	1.0%	0.601	0.1%	0.01
202	p-SnTeSb_0.04	475	44	0.32	4.86	0.06	1.4%	1.37	1.7228	1.3%	0.601	0.2%	0.02
227	p-SnTeSb_0.04	500	49	0.35	4.66	0.07	1.8%	1.47	1.7321	1.7%	0.602	0.3%	0.02
252	p-SnTeSb_0.04	525	54	0.38	4.45	0.09	2.2%	1.58	1.7426	2.2%	0.602	0.4%	0.03
277	p-SnTeSb_0.04	550	60	0.41	4.25	0.11	2.7%	1.68	1.7543	2.7%	0.603	0.5%	0.03
302	p-SnTeSb_0.04	575	66	0.44	4.04	0.14	3.3%	1.79	1.7676	3.3%	0.604	0.6%	0.04
327	p-SnTeSb_0.04	600	73	0.48	3.83	0.17	4.0%	1.90	1.7823	4.0%	0.605	0.8%	0.05
352	p-SnTeSb_0.04	625	80	0.52	3.61	0.21	4.8%	2.01	1.7988	4.7%	0.606	0.9%	0.05
377	p-SnTeSb_0.04	650	87	0.57	3.40	0.25	5.7%	2.12	1.8172	5.5%	0.607	1.1%	0.06
402	p-SnTeSb_0.04	675	95	0.62	3.19	0.31	6.7%	2.22	1.8375	6.5%	0.608	1.4%	0.07
427	p-SnTeSb_0.04	700	103	0.68	2.98	0.37	7.8%	2.33	1.8602	7.5%	0.610	1.6%	0.08
452	p-SnTeSb_0.04	725	112	0.75	2.77	0.44	9.0%	2.45	1.8852	8.6%	0.612	1.9%	0.10
477	p-SnTeSb_0.04	750	121	0.83	2.55	0.52	10.4%	2.57	1.9130	9.9%	0.614	2.2%	0.11
502	p-SnTeSb_0.04	775	131	0.91	2.34	0.62	12.0%	2.70	1.9438	11.2%	0.616	2.5%	0.12

S.3.6 Spreadsheet for the calculation of ZT for $SnTeSb_{0.045}$

T (C)	Material	*T* (K)	Seebeck (μV/K)	resistivity (10-3 Ω cm)	thermal cond (W/m K)	*zT*	max red eff	*s* (1/V)	*u* (1/V)	red eff	Φ (V)	efficiency	*ZT*
27	p-SnTeSb_0.045	300	20	0.17	6.31	0.01	0.3%	0.92	1.8302	0.0%	0.552		
52	p-SnTeSb_0.045	325	22	0.18	6.09	0.01	0.4%	0.98	1.8341	0.1%	0.552	0.0%	0.00
77	p-SnTeSb_0.045	350	24	0.20	5.88	0.02	0.4%	1.04	1.8383	0.2%	0.552	0.0%	0.00
102	p-SnTeSb_0.045	375	27	0.21	5.67	0.02	0.6%	1.11	1.8433	0.3%	0.553	0.0%	0.01
127	p-SnTeSb_0.045	400	30	0.23	5.47	0.03	0.7%	1.19	1.8493	0.5%	0.553	0.1%	0.01
152	p-SnTeSb_0.045	425	33	0.25	5.26	0.04	0.9%	1.28	1.8562	0.7%	0.553	0.1%	0.01
177	p-SnTeSb_0.045	450	37	0.26	5.04	0.05	1.1%	1.38	1.8642	1.0%	0.553	0.1%	0.01
202	p-SnTeSb_0.045	475	42	0.29	4.82	0.06	1.4%	1.48	1.8735	1.3%	0.554	0.2%	0.02
227	p-SnTeSb_0.045	500	46	0.31	4.62	0.07	1.8%	1.59	1.8840	1.7%	0.554	0.3%	0.02
252	p-SnTeSb_0.045	525	52	0.34	4.41	0.09	2.2%	1.69	1.8961	2.2%	0.554	0.4%	0.03
277	p-SnTeSb_0.045	550	57	0.37	4.21	0.12	2.8%	1.80	1.9097	2.8%	0.555	0.5%	0.03
302	p-SnTeSb_0.045	575	63	0.40	4.00	0.14	3.4%	1.91	1.9251	3.4%	0.556	0.6%	0.04
327	p-SnTeSb_0.045	600	70	0.44	3.79	0.18	4.1%	2.03	1.9425	4.1%	0.557	0.8%	0.05
352	p-SnTeSb_0.045	625	77	0.48	3.58	0.22	4.9%	2.15	1.9619	4.9%	0.558	1.0%	0.06
377	p-SnTeSb_0.045	650	84	0.52	3.38	0.26	5.8%	2.27	1.9836	5.8%	0.559	1.2%	0.07
402	p-SnTeSb_0.045	675	92	0.57	3.18	0.32	6.9%	2.39	2.0079	6.8%	0.560	1.4%	0.08
427	p-SnTeSb_0.045	700	101	0.62	2.98	0.39	8.1%	2.52	2.0350	7.9%	0.562	1.7%	0.09
452	p-SnTeSb_0.045	725	109	0.67	2.78	0.47	9.5%	2.66	2.0652	9.1%	0.563	2.0%	0.10
477	p-SnTeSb_0.045	750	119	0.72	2.58	0.56	11.1%	2.82	2.0988	10.5%	0.565	2.3%	0.11
502	p-SnTeSb_0.045	775	128	0.78	2.38	0.69	13.0%	3.01	2.1361	12.1%	0.567	2.7%	0.13

S.3.7 Spreadsheet for the calculation of ZT for $SnTeSb_{0.05}$

T (C)	Material	*T* (K)	Seebeck (μV/K)	resistivity (10-3 Ω cm)	thermal cond (W/m K)	*zT*	max red eff	*s* (1/V)	*u* (1/V)	red eff	Φ (V)	efficiency	*ZT*
27	p-SnTeSb_0.05	300	17	0.15	6.94	0.01	0.2%	0.78	1.8677	-0.2%	0.540		
52	p-SnTeSb_0.05	325	19	0.17	6.66	0.01	0.3%	0.87	1.8721	-0.1%	0.540	0.0%	-0.01
77	p-SnTeSb_0.05	350	22	0.18	6.41	0.01	0.4%	0.95	1.8768	0.0%	0.540	0.0%	0.00
102	p-SnTeSb_0.05	375	25	0.19	6.15	0.02	0.5%	1.04	1.8825	0.2%	0.540	0.0%	0.00
127	p-SnTeSb_0.05	400	28	0.20	5.90	0.03	0.6%	1.14	1.8891	0.4%	0.541	0.0%	0.00
152	p-SnTeSb_0.05	425	32	0.22	5.66	0.03	0.8%	1.26	1.8968	0.6%	0.541	0.0%	0.00
177	p-SnTeSb_0.05	450	36	0.24	5.40	0.05	1.1%	1.38	1.9057	0.9%	0.541	0.1%	0.01
202	p-SnTeSb_0.05	475	41	0.26	5.15	0.06	1.4%	1.50	1.9159	1.3%	0.541	0.1%	0.01
227	p-SnTeSb_0.05	500	46	0.28	4.92	0.08	1.8%	1.63	1.9276	1.8%	0.542	0.2%	0.02
252	p-SnTeSb_0.05	525	51	0.31	4.68	0.10	2.3%	1.76	1.9409	2.3%	0.542	0.3%	0.02
277	p-SnTeSb_0.05	550	57	0.33	4.46	0.12	2.9%	1.88	1.9560	2.9%	0.543	0.4%	0.03
302	p-SnTeSb_0.05	575	64	0.36	4.23	0.15	3.6%	2.01	1.9730	3.6%	0.544	0.6%	0.04
327	p-SnTeSb_0.05	600	71	0.40	4.00	0.19	4.3%	2.13	1.9921	4.3%	0.545	0.8%	0.05
352	p-SnTeSb_0.05	625	78	0.44	3.77	0.23	5.2%	2.26	2.0136	5.2%	0.546	0.9%	0.06
377	p-SnTeSb_0.05	650	86	0.48	3.56	0.28	6.3%	2.38	2.0376	6.1%	0.547	1.2%	0.07
402	p-SnTeSb_0.05	675	95	0.52	3.35	0.34	7.4%	2.50	2.0645	7.2%	0.548	1.4%	0.08
427	p-SnTeSb_0.05	700	103	0.57	3.15	0.41	8.6%	2.62	2.0946	8.3%	0.550	1.7%	0.09
452	p-SnTeSb_0.05	725	113	0.63	2.94	0.50	10.1%	2.74	2.1282	9.6%	0.552	2.0%	0.10
477	p-SnTeSb_0.05	750	122	0.68	2.74	0.60	11.6%	2.87	2.1657	11.1%	0.553	2.3%	0.12
502	p-SnTeSb_0.05	775	132	0.74	2.55	0.72	13.4%	3.02	2.2075	12.6%	0.556	2.7%	0.13