Thermoelectric properties of half-Heusler high-entropy $Ti_2NiCoSn_{1-x}Sb_{1+x}$ (x=0.5, 1) alloys with VEC>18

Anirudha Karati[1], V.S. Hariharan[2], Sanyukta Ghosh[3], Anil Prasad[4], M. Nagini[2], K. Guruvidyathri[5], Ramesh Chandra Mallik[3], Rajashekhara Shabadi[6], Lukas Bichler[4], B.S. Murty[2*], U.V. Varadaraju[1]

[1]Department of Chemistry, [2]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India

[3]Thermoelectric Materials and Devices Laboratory, Department of Physics, Indian Institute of Science, Bangalore, India

[4]School of Engineering University of British Columbia Okanagan, Kelowna, Canada

[5]School of Engineering Sciences and Technology, University of Hyderabad, Gachibowli, Hyderabad, India

[6]Faculty of Science and Technology, UMET, University of Lille, Villeneuve-d'Ascq, France

*Corresponding author

Email address: murty@iitm.ac.in

Supplementary Data

Table S1: Precision lattice parameter of $Ti_2NiCoSn_{1-x}Sb_{1+x}$alloys synthesized by various processing routes. The alloy x=0 has been reported in [14].

Alloy (x)	Lattice parameter (nm)	
	Cast	1h BM-SPS
0	0.5915	0.5904
0.5	0.5898	0.5885
1	0.5892	0.5881

Table S2: SEM-EDS compositional analysis in $Ti_2NiCoSn_{1-x}Sb_{1+x}$as-cast alloys (N=3). The alloy x=0 has been reported in [14].

Alloy (x)	Phase	Element					
		Ti	Ni	Co	Sn	Sb	O
	Expected	33.3	16.6	16.6	16.6	16.6	0
	Overall	36.9±0.4	16.2±0.1	17.4±0.0	13.8±0.2	15.7±0.2	0

0	Grey	33.3±1.6	19.6±0.3	16.2±0.5	14.4±0.7	16.4±0.1	0
	White	0	0	0	100	0	0
	Black	83.4±2.4	2.6±0.3	3.2±1.1	7.7±0.6	3.1±0.3	0
	Expected	33.3	16.6	16.6	8.3	25	0
	Overall	34.2±0.3	15.5±0.3	16.5±0.3	8.4±0.2	25.4±0.2	0
0.5	Grey	33.0±0.3	17.1±0.4	18.6±0.1	8.7±0.4	22.5±0.5	0
	White	2.2±0.3	0.9±0.0	0.1±0.0	52.9±0.3	43.8±0.6	0
	Black	55.7±0.6	3.4±0.2	3.1±0.2	2.8±0.2	3.5±0.4	31.5±0.9
	Expected	33.3	16.6	16.6	0	33.3	0
	Overall	34.0±0.4	16.3±0.9	15.8±0.7	0	34.0±0.6	0
1	Grey	33.3±0.1	16.1±1.5	15.4±1.6	0	35.2±1.2	0
	White	0	29.0±1.2	0	0	71.0±1.2	0
	Black	55.4±1.7	0.7±0.6	0.4±0.3	0	2.1±1.5	41.4±4.1

Table S3: Entropy calculation

Sample	ΔS_{config}
$Ti_2NiCoSnSb$	$-R\left(\frac{2}{6}(0)+\frac{2}{6}\left(\frac{1}{2}ln\frac{1}{2}+\frac{1}{2}ln\frac{1}{2}\right)+\frac{2}{6}\left(\frac{1}{2}ln\frac{1}{2}+\frac{1}{2}ln\frac{1}{2}\right)\right)$
$Ti_2NiCoSn_{0.5}Sb_{1.5}$	$-R\left(\frac{2}{6}(0)+\frac{2}{6}\left(\frac{1}{2}ln\frac{1}{2}+\frac{1}{2}ln\frac{1}{2}\right)+\frac{2}{6}\left(\frac{0.5}{2}ln\frac{0.5}{2}+\frac{1.5}{2}ln\frac{1.5}{2}\right)\right)$
$Ti_2NiCoSb_2$	$-R\left(\frac{2}{6}(0)+\frac{2}{6}\left(\frac{1}{2}ln\frac{1}{2}+\frac{1}{2}ln\frac{1}{2}\right)+\frac{2}{6}(0)\right)$
TiNiSn	$-R\left(\frac{2}{6}(0)+\frac{2}{6}(0)+\frac{2}{6}(0)\right)$
TiCoSb	$-R\left(\frac{2}{6}(0)+\frac{2}{6}(0)+\frac{2}{6}(0)\right)$

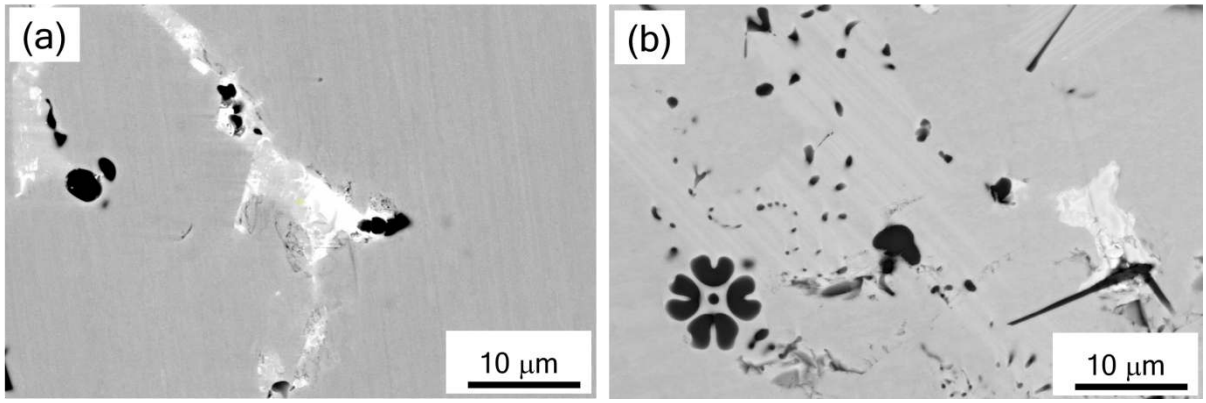

Figure S1: BSE images of as-cast $Ti_2NiCoSn_{1-x}Sb_{1+x}$ where (a) x=0.5, (b) x=1 alloys.

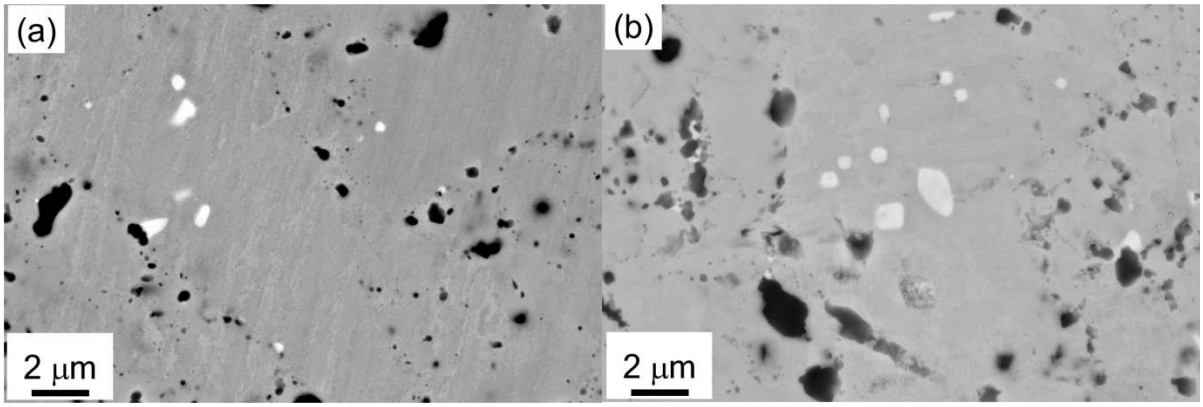

Figure S2: BSE images of 1h BM-SPS $Ti_2NiCoSn_{1-x}Sb_{1+x}$ where (a) x=0.5, (b) x=1 alloys.

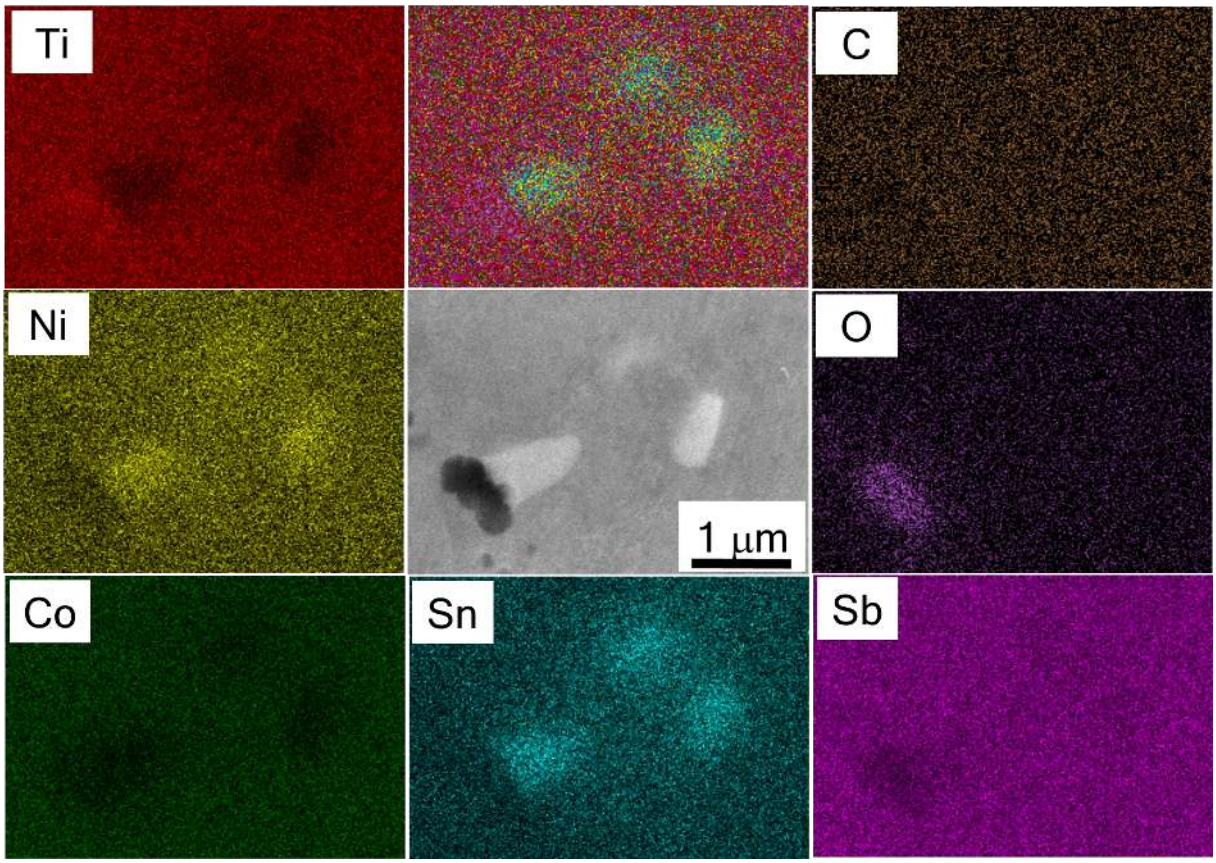

Figure S3: Elemental map of 1h BM-SPS $Ti_2NiCoSn_{0.5}Sb_{1.5}$ alloy.

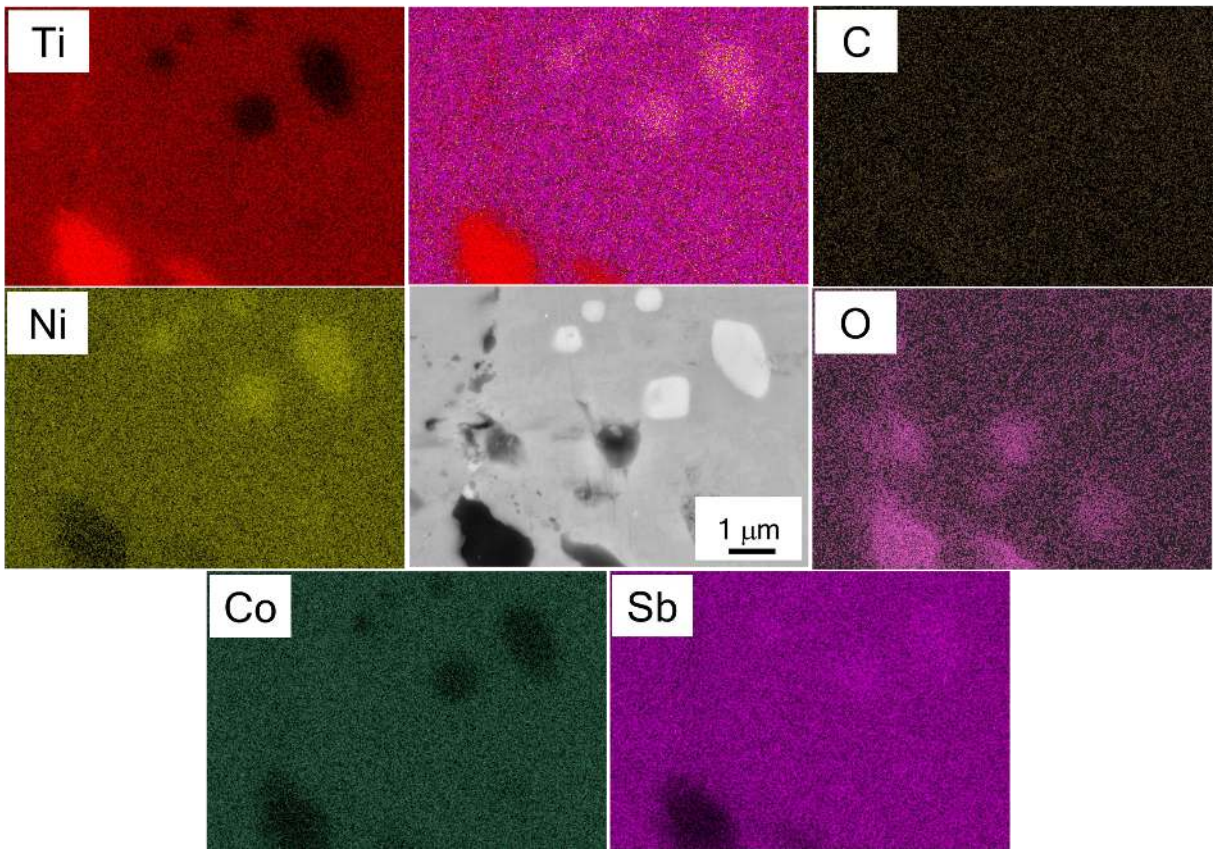

Figure S4: Elemental map of 1h BM-SPS $Ti_2NiCoSb_2$ alloy.

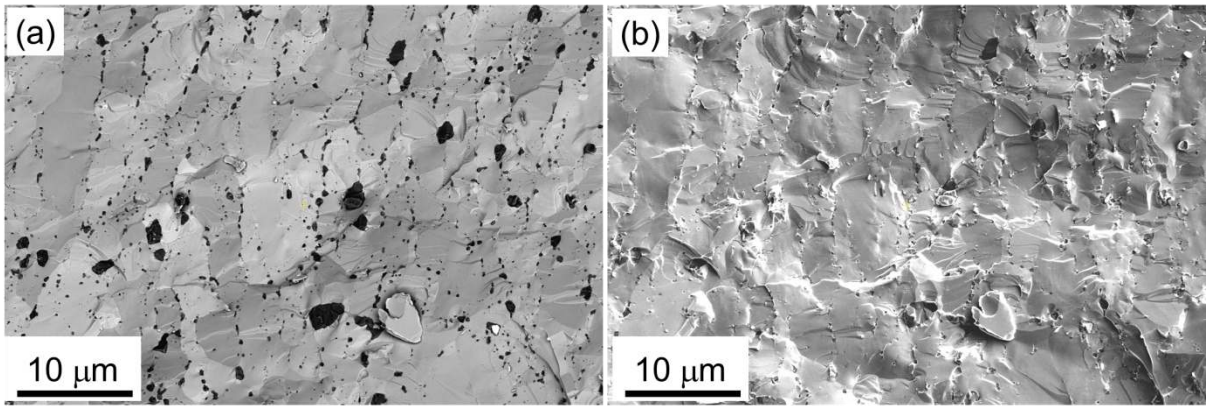

Figure S5: (a) BSE and (b) SE images of the fractured surface of 1h BM-SPS $Ti_2NiCoSn_{0.5}Sb_{1.5}$ alloy showing presence of TiO_2 at the grain boundaries.