Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Supporting Information for

Thermoelectric Performance of Multiphase XNiSn (X = Ti, Zr, Hf) half-Heusler Alloys

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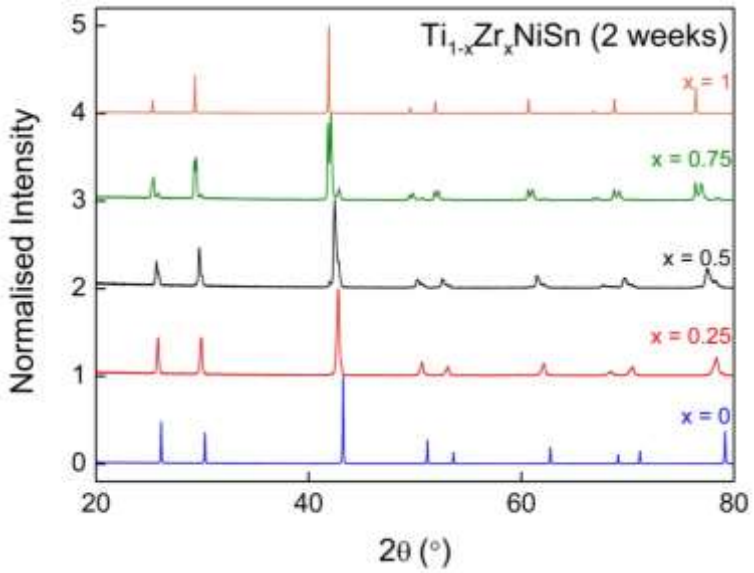

Fig. S1(a). Laboratory X-ray powder diffraction data for the $Ti_{1-x}Zr_xNiSn$ series

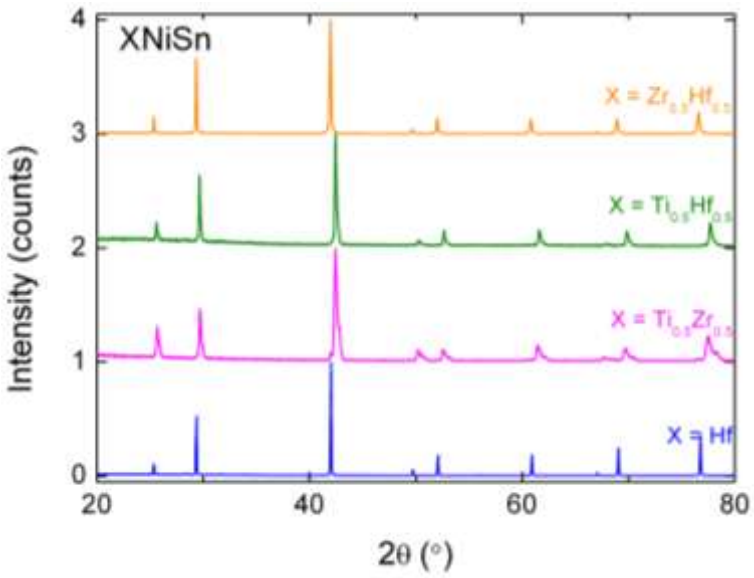

Fig. S1(b). Laboratory X-ray powder diffraction data for the XNiSn series (X = Hf, $Ti_{0.5}Zr_{0.5}$, $Ti_{0.5}Hf_{0.5}$ and $Zr_{0.5}Hf_{0.5}$).

Table S1. Nominal compositions, anneal time, lattice parameter (a), experimental compositions (using Vegard's law – x_{veg}), composition variance (Δx), molar percentages (mol%), average composition (x_{avg}) , and goodness of fit (χ^2) for the $Ti_{1-x}Zr_xNiSn_{0.95}$ compositions.

x	Anneal Time	a (Å)	x_{vegard}	Δx	mol%	x_{avg}	χ^2
0	3 days	5.9282(1)		0	79(1)		2.9
		5.9319(1)	N/A	0	21(1)	N/A	
	6 weeks	5.9325(1)		0	50		1.8
		5.9355(1)		0.02(1)	50		
0.025	3 days	5.9313(1)	0.02(1)	0.01(1)	73(1)	0.023	2.9
		5.9351(1)	0.04(1)	0.01(1)	27(1)		
0.05	3 days	5.9331(1)	0.03(1)	0.01(1)	38.4(9)	0.05	3.1
		5.9390(1)	0.06(1)	0.03(1)	61.6(9)		
	6 weeks	5.9410(1)	0.05(1)	0.01(1)	45(2)	0.07	1.5
		5.9462(1)	0.08(1)	0.05(1)	55(2)		
0.25	3 days	5.9393(1)	0.06(1)	-0.01(1)	2.5(8)		
		5.9722(1)	0.25(1)	0.16(1)	78.0(6)	0.27	3.3
		5.9974(1)	0.39(1)	0.11(1)	19.6(5)		
	6 weeks	5.9654(1)	0.19(1)	0.04(1)	22.0(6)		
		5.9748(1)	0.24(1)	0.09(1)	56.5(3)	0.25	1.9
		5.9908(1)	0.33(1)	0.15(1)	20.4(5)		
		6.0749(1)	0.81(1)	0.07(4)	1.1(1)		
0.5	3 days	5.9786(1)	0.28(1)	0.23(1)	16.7(2)		
		6.0221(1)	0.53(1)	0.21(1)	62.2(1)	0.57	2.9
		6.0856(1)	0.88(1)	0.11(1)	4.8(2)		
		6.1041(1)	0.98(1)	0.05(1)	16.3(3)		
	1 week	5.9917(1)	0.38(1)	0.09(1)	10.8(3)		
		6.0108(1)	0.46(1)	0.15(1)	56.6		
		6.0289(1)	0.56(1)	0.15(1)	21.6(3)	0.56	2.2
		6.0820(1)	0.86(1)	0.07(1)	3.8(2)		
		6.1016(1)	0.97(1)	0.10(1)	7.1(2)		
	2 weeks	6.0029(1)	0.43(1)	0.08(1)	16.7(5)		
		6.0170(1)	0.49(1)	0.10(1)	24.2(4)		
		6.0292(1)	0.56(1)	0.10(1)	46.7	0.56	1.7
		6.0837(1)	0.87(1)	0.13(1)	8.7(3)		
		6.1020(1)	0.97(1)	0.08(1)	3.7(2)		
	3 weeks	6.0034(1)	0.43(1)	0.11(1)	20.1(6)		
		6.0182(1)	0.50(1)	0.10(1)	26.1(4)		
		6.0306(1)	0.57(1)	0.10(1)	46.2	0.55	1.6
		6.0838(1)	0.87(1)	0.05(1)	3.8(2)		
		6.1006(1)	0.97(1)	0.08(1)	3.7(2)		
	4 weeks	6.0177(1)	0.49(1)	0.09(1)	29.1		
		6.0320(1)	0.58(1)	0.10(1)	63.7(8)	0.57	1.9
		6.0880(1)	0.88(1)	0.19(1)	7.3(2)		
	6 weeks	6.0076(1)	0.44(1)	0.07(1)	24.5(7)		
		6.0194(1)	0.49(1)	0.09(1)	36.7(6)	0.52	1.5
		6.0302(1)	0.55(1)	0.09(1)	32.9(9)		
		6.0867(1)	0.89(1)	0.07(1)	6.0(2)		
0.5	Arc-melted	5.9891(1)	0.32(1)	0.20(2)	16.8(4)		
		6.0264(1)	0.52(1)	0.56(4)	19.9(9)	0.61	2.4
		6.0612(1)	0.71(1)	0.11(1)	63.2(2)		
0.75	3 days	6.0394(1)	0.62(1)	0.33(1)	21.4(5)		
		6.0871(1)	0.89(1)	0.16(1)	20.6(8)	0.89	4.3
		6.1053(1)	0.99(1)	0.03(1)	58.0(6)		
	6 weeks	6.0798(1)	0.84(1)	0.07(1)	67.1(3)	0.88	1.6
		6.1022(1)	0.97(1)	0.09(1)	32.8(3)		
1.0	3 days	6.1075(1)	N/A	0.01(1)	100	N/A	5.7
	6 weeks	6.1080(1)		0	100		1.9
0.5, 0.025	4 weeks	6.0003(1)	0.39(1)		22	0.505	1.6
		6.0088(1)	0.44(1)		8		
		6.0193(1)	0.49(1)		49		
		6.0278(1)	0.54(1)		12		
		6.0844(3)	0.87(1)		5		
		6.1001(5)	0.96(1)		4		

6 weeks: $\Delta x = 0.3380 \Delta d/d$; 3 days: $\Delta x = 0.3306 \Delta d/d$. Arc-melted sample reported in Downie et al. Chemical Communications 49, 4184 (2013).

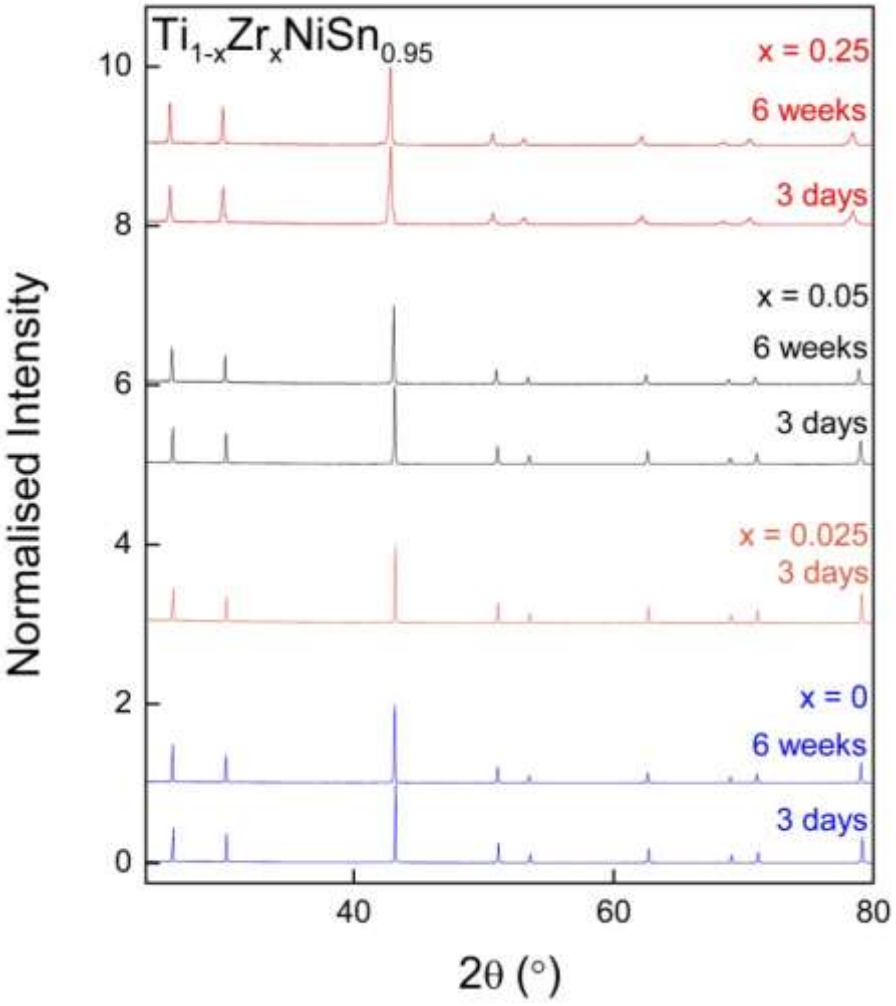

Fig. S2(a). Laboratory X-ray powder diffraction patterns for the $Ti_{1-x}Zr_xNiSn_{0.95}$ series ($0 \leq x \leq 0.25$).

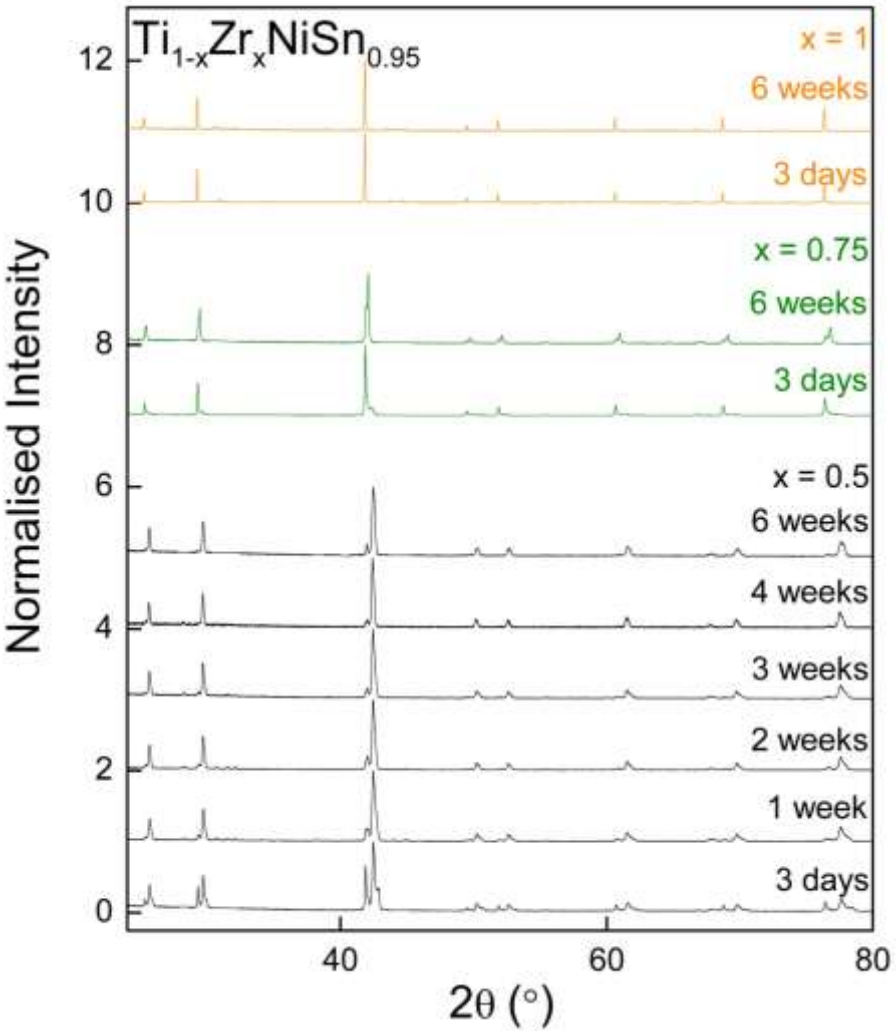

Fig. S2(b). Laboratory X-ray powder diffraction patterns for the $Ti_{1-x}Zr_xNiSn_{0.95}$ series ($0.5 \leq x \leq 1$).

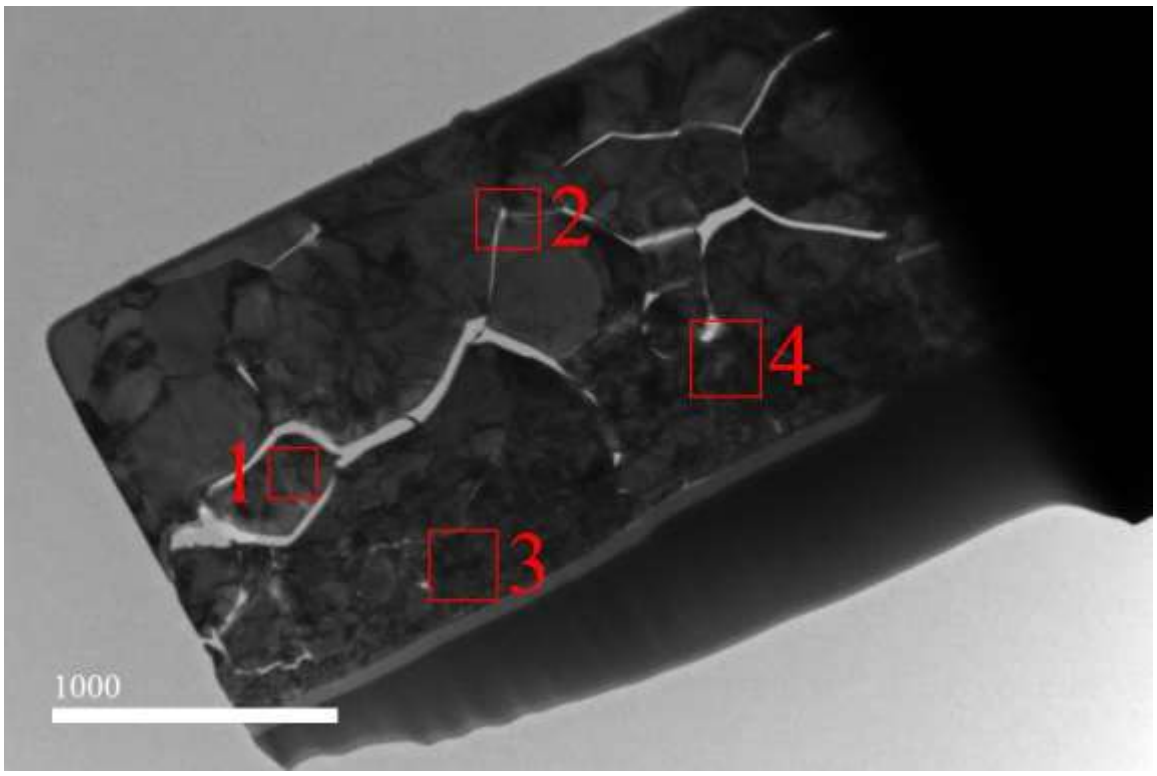

Fig. S3. A low magnification image of the FIB lamella prepared from the $Ti_{0.5}Zr_{0.5}NiSn$ pellet. Areas 1-4 were studied using TEM and EDX mapping (Fig. 2 in the manuscript). The sample area is approximately 2.5 x 5 μm^2.

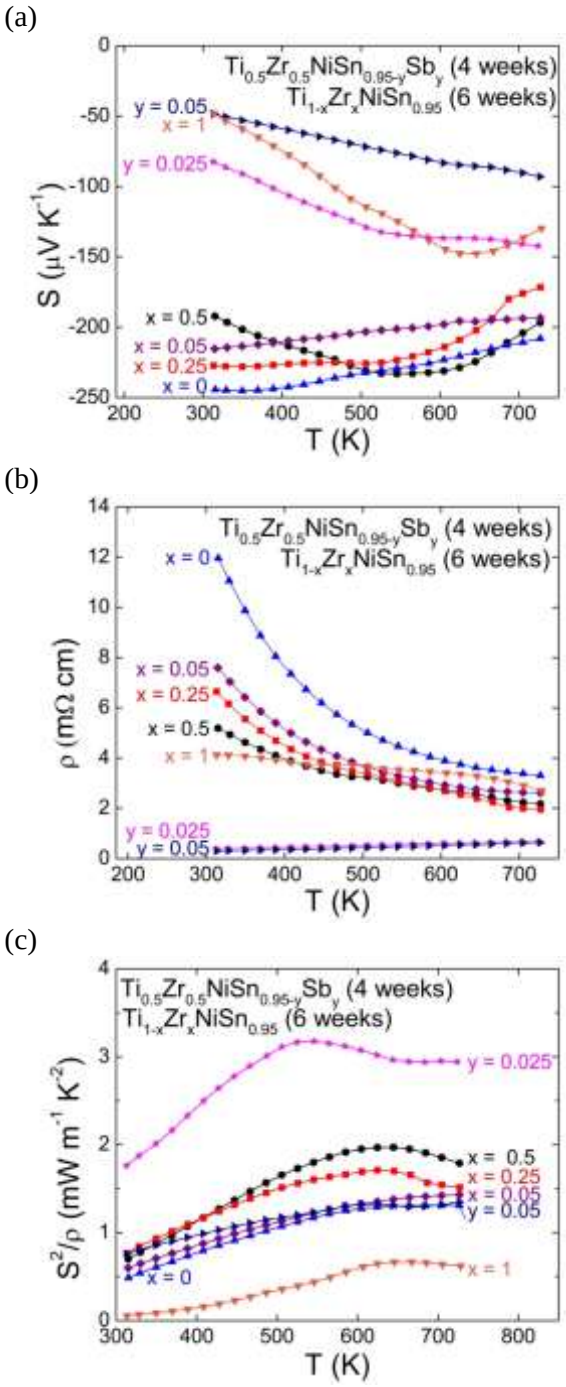

Fig. S4. Temperature dependence of the (a) Seebeck coefficient, (b) electrical resistivity and (c) power factor for the $Ti_{1-x}Zr_xNiSn_{0.95-y}Sb_y$ series.