Band structure modification of the thermoelectric Heusler-phase $TiFe_2Sn$ via Mn substitution

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1. Rietveld refinement results

Table S1 Results of Le Bail refinements of powder X-ray diffraction data of $TiFe_{2-x}Mn_xSn$.

Mn content/x	Unit cell parameter a / Å	R_p / %	R_{wp} / %	R_{Bragg} / %	χ^2
0	6.0623(7)	4.35	5.68	1.06	1.50
0.01	6.0602(7)	4.02	5.12	1.47	1.32
0.0156	6.0557(7)	4.31	5.52	1.77	1.31
0.0185	6.0549(7)	4.17	5.26	1.43	1.28
0.02	6.0584(7)	4.26	5.49	1.37	1.42
0.03	6.0593(7)	4.22	5.46	1.45	1.71
0.05	6.0614(7)	4.45	5.7	1.22	1.36

The Rietveld refinement results show that the deviation of lattice parameter is in the area of about 0.1% among all $TiFe_{2-x}Mn_xSn$ samples. It should be kept in mind that minor variations of the Ti and Sn contents will strongly influence the detected unit cell parameters of the Full-Heusler phase $TiFe_{2-x}Mn_xSn$, as observed from the formation of small amounts of secondary phases (e.g. TiO_2 and Sn, s. Figure S1 and Figure S2). Typically, very weak reflections for the secondary phases were observed, because the impurity phase content was close to detection limit of our X-ray diffractometer. A significant amount of TiO_2 was only recognized in the sample $x = 0.0156$. On the other hand, Rietveld refinements of the collected diffraction data (s. Figure S1) to determine the actual phase compositions were strongly hampered by the observed X-ray fluorescence generated by the interaction of Cu-K_α radiation with Fe and Mn atoms, respectively, leading to an increased measurement background, especially at higher 2Θ angles and the small quantities of impurity phases.

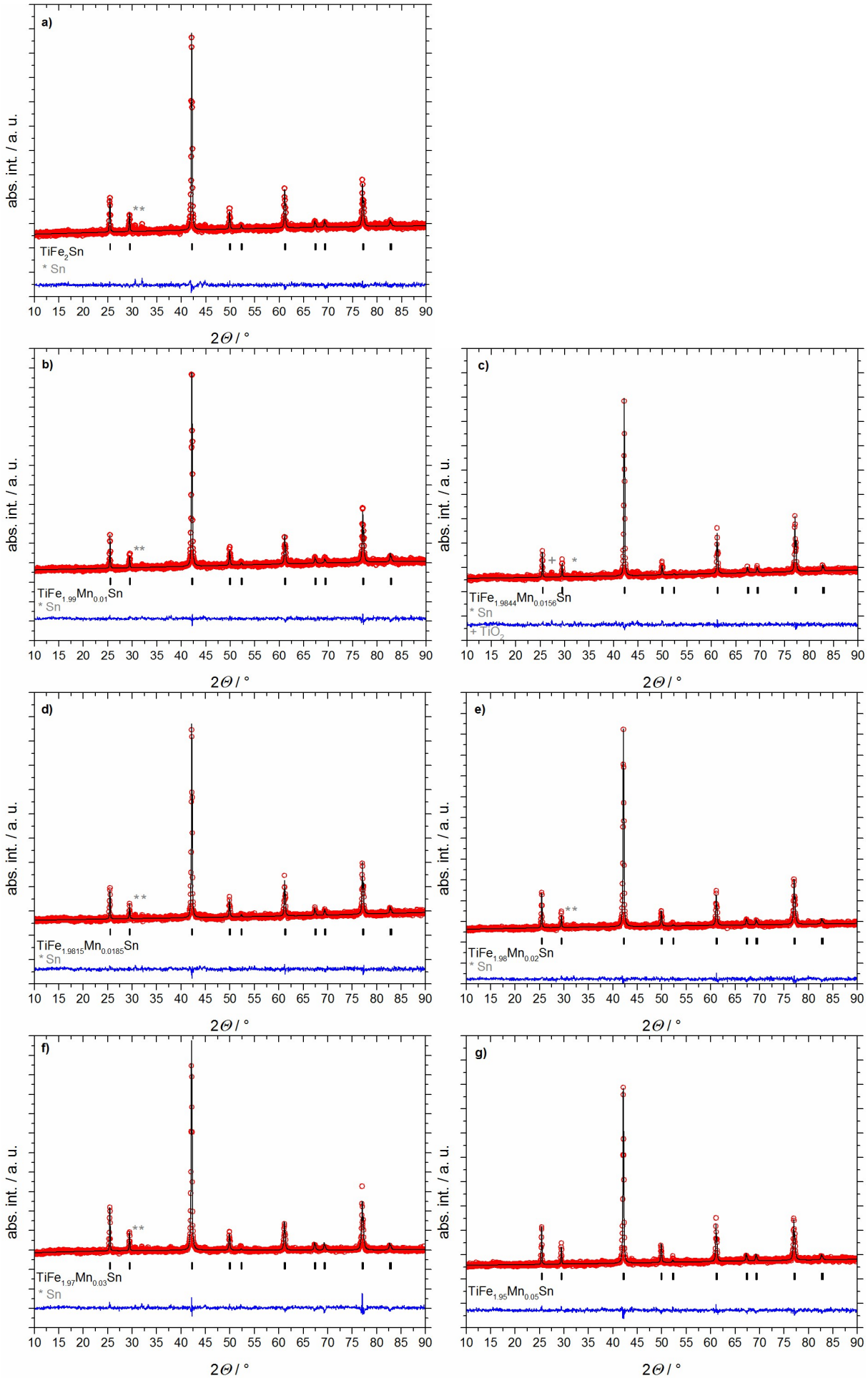

Figure S1 Le Bail refinements of the powder X-ray diffraction data of a) $TiFe_2Sn$, b) $TiFe_{1.99}Mn_{0.01}Sn$, c) $TiFe_{1.9844}Mn_{0.0156}Sn$, d) $TiFe_{1.9815}Mn_{0.0185}Sn$, e) $TiFe_{1.98}Mn_{0.02}Sn$, f) $TiFe_{1.97}Mn_{0.03}Sn$, and g) $TiFe_{1.95}Mn_{0.05}Sn$.

2. SEM image

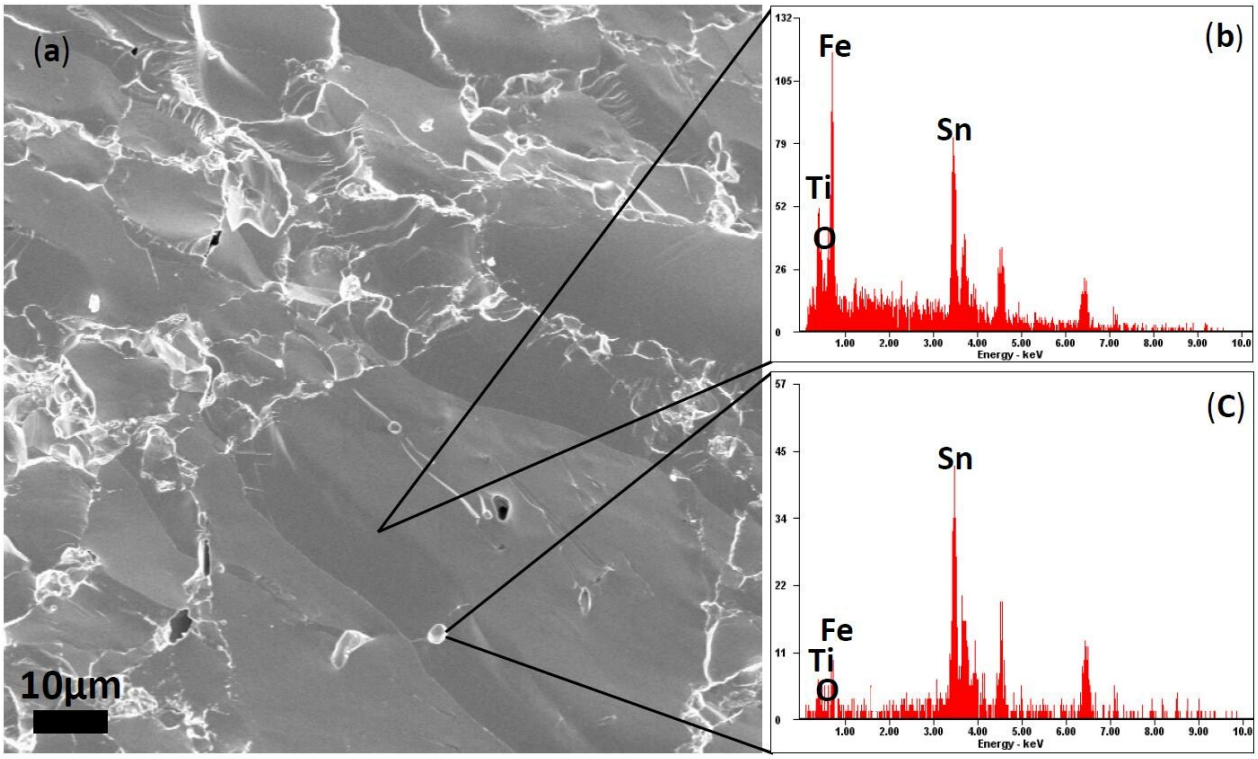

Figure S2. (a)Typical scanning electronic microscopy image of $TiFe_2Sn$ sample. (b) An energy dispersive X-ray spectrum (EDS) of the matrix. (c) EDS of an impurity particle in the compound.

3. Total DOS of $TiFe_2Sn$ compound

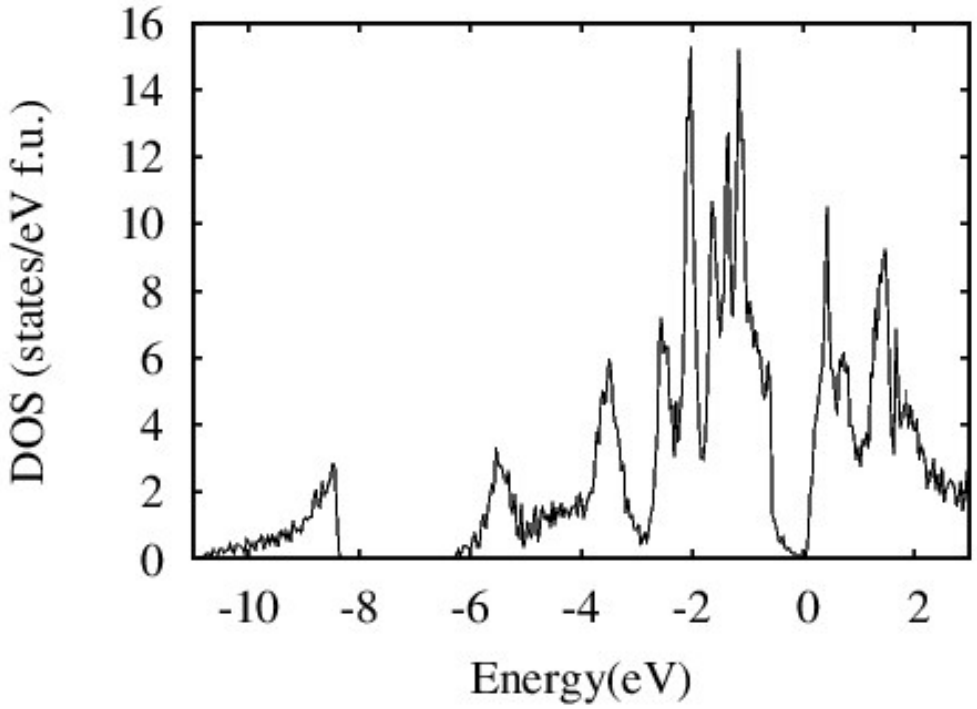

Figure S3. The total DOS of $TiFe_2Sn$ using the states/eV*fu unit, the large energy scale (-11eV, 3eV) and smaller smearing value.