Supporting Information

Solubility limits in quaternary SnTe-based alloys

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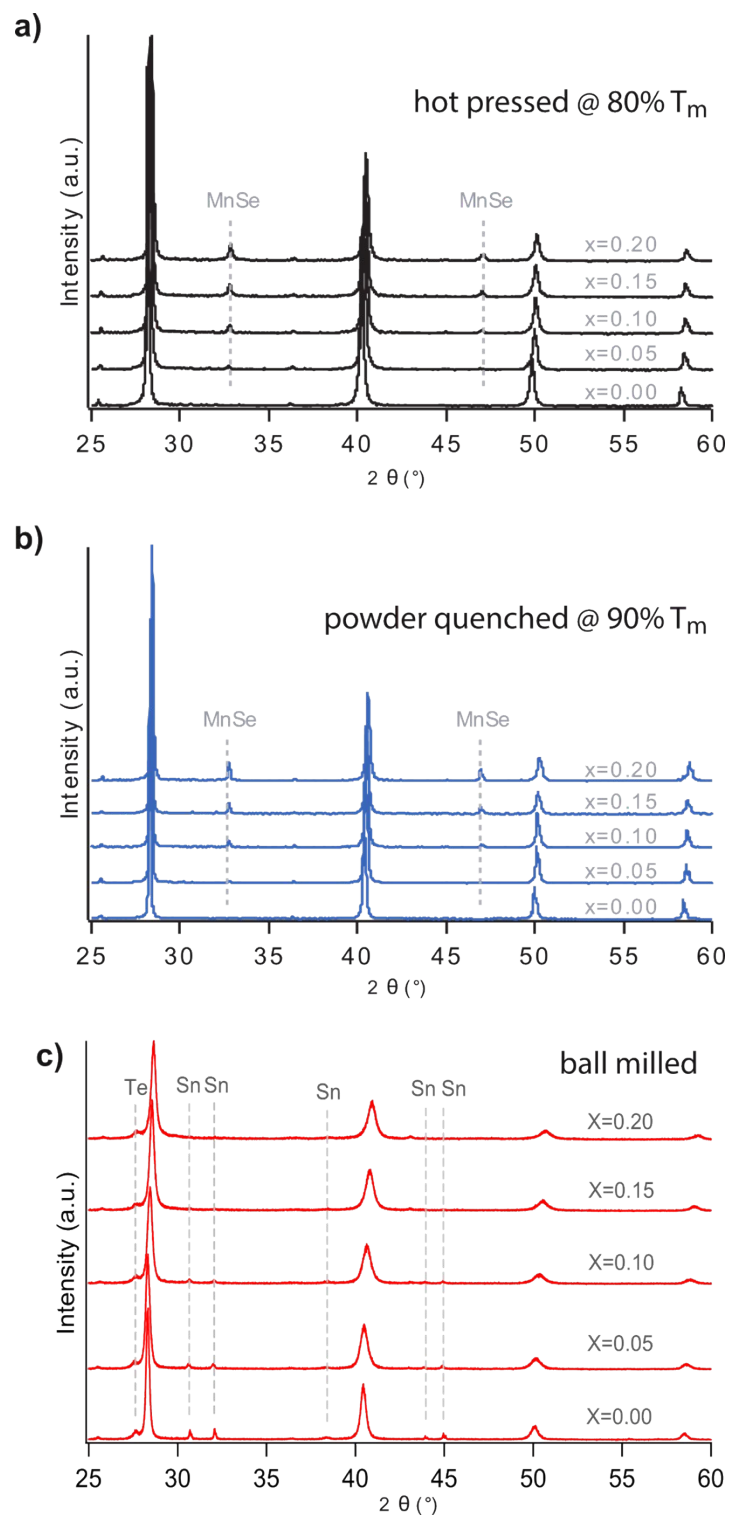
Figure S1: Detailed XRD analysis for $Sn_{1-x}Mn_xSe_{1-x}Te_x$ alloys synthesized by different equilibrium and non-equilibrium methods. For the ball-milled powders Sn (PDF# 04-0673) as well as Te (PDF# 36-1452) impurities are present.
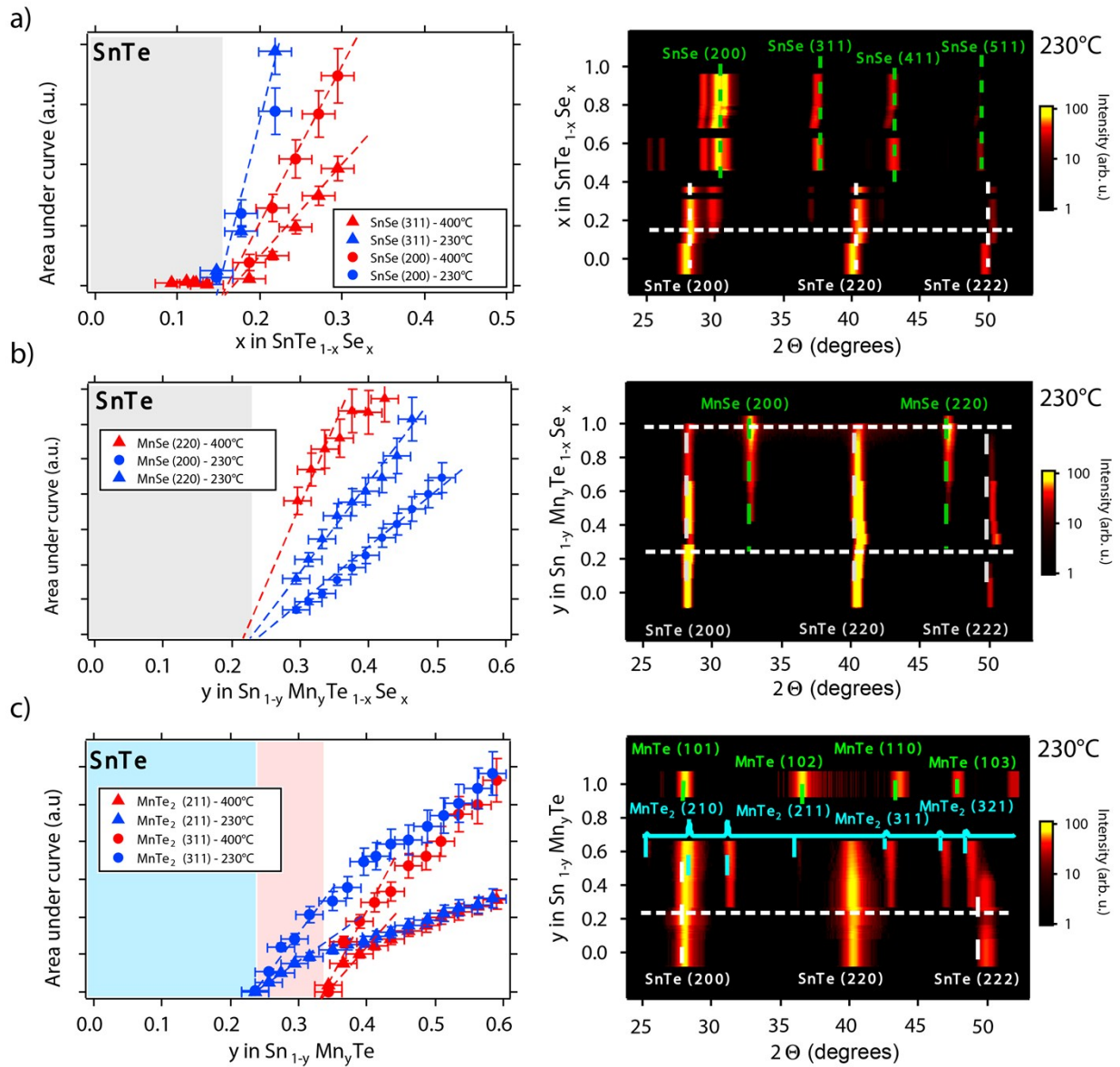
Figure S2: Disappearing phase method analysis for the determination of non-equilibrium solubility limits with the corresponding false color XRD plots a) Alloying of SnTe and SnSe b) Alloying SnTe and MnSe c) Alloying of SnTe and MnTe
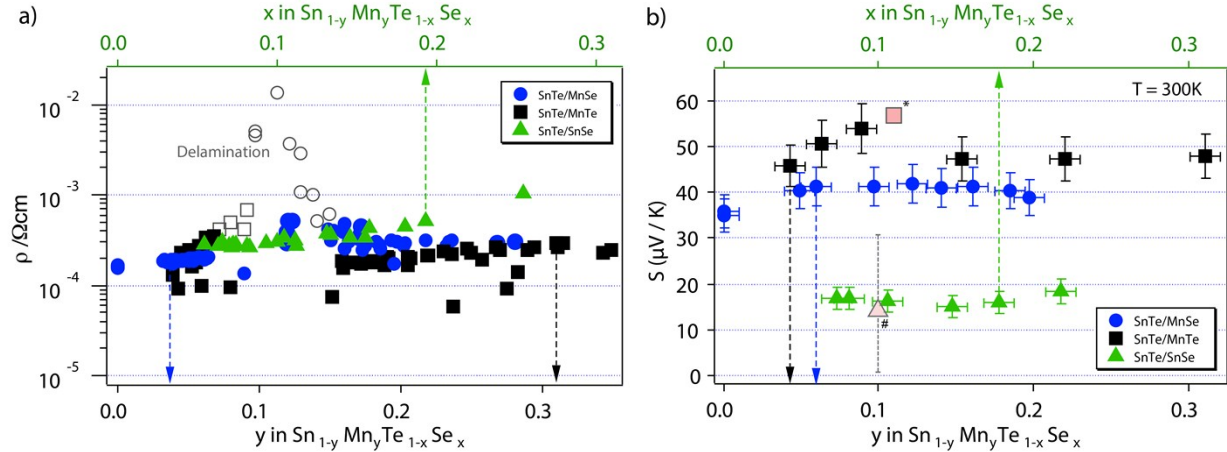
Figure S3: Screening of the electrical properties of SnTe alloys. a) Resistivity of the films ρ measured with 4pp mapping. A slight increase resistivity can be observed with increased alloying concentration for all alloying experiments. For several libraries, delamination of the films lead to increased resistivities. b) Measurements of the Seebeck coefficient S at 300K. The measurements were carried out on individual samples. Literature values for measurements of $Sn_{0.89}Mn_{0.11}Te$ (*,) and $SnTe_{0.90}Se_{0.10}$ (#) at 300K are displayed for comparison[1–3].

References:

1   G. Tan, F. Shi, S. Hao, H. Chi, T. P. Bailey, L.-D. Zhao, C. Uher, C. Wolverton, V. P. Dravid and M. G. Kanatzidis, *J. Am. Chem. Soc.*, 2015, 150826160359004.

2   L. Wang, S. Zheng and H. Chen, *J. Electron. Mater.*, 2016.

3   A. Banik and K. Biswas, *J. Mater. Chem. A*, 2014, **2**, 9620.