

Supplementary Information for

Layered germanium tin antimony tellurides: element distribution, nanostructures and thermoelectric properties

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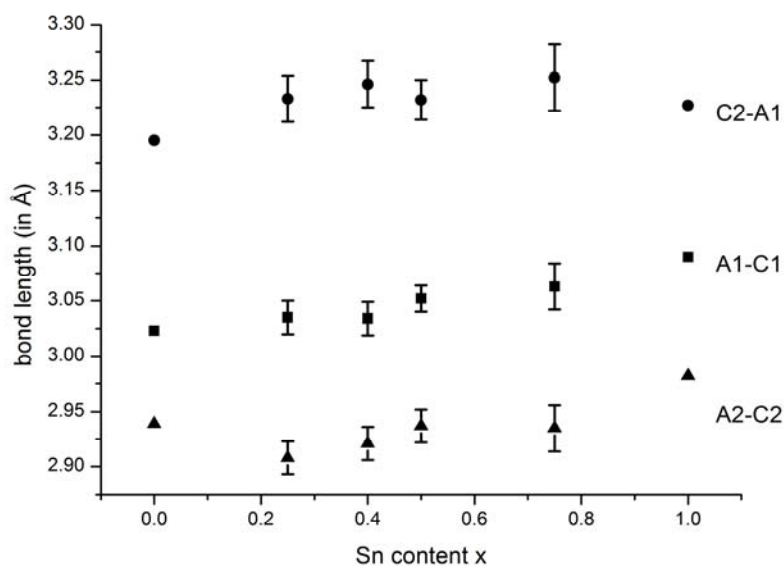


Figure S1: Trend of the cation-anion bond lengths (labelling cf. Fig. 4) with increasing Sn content x ; error bars correspond to 3 standard deviations; bond lengths for GeSb_2Te_4 and SnSb_2Te_4 taken from literature (refs. [20] and [22]).

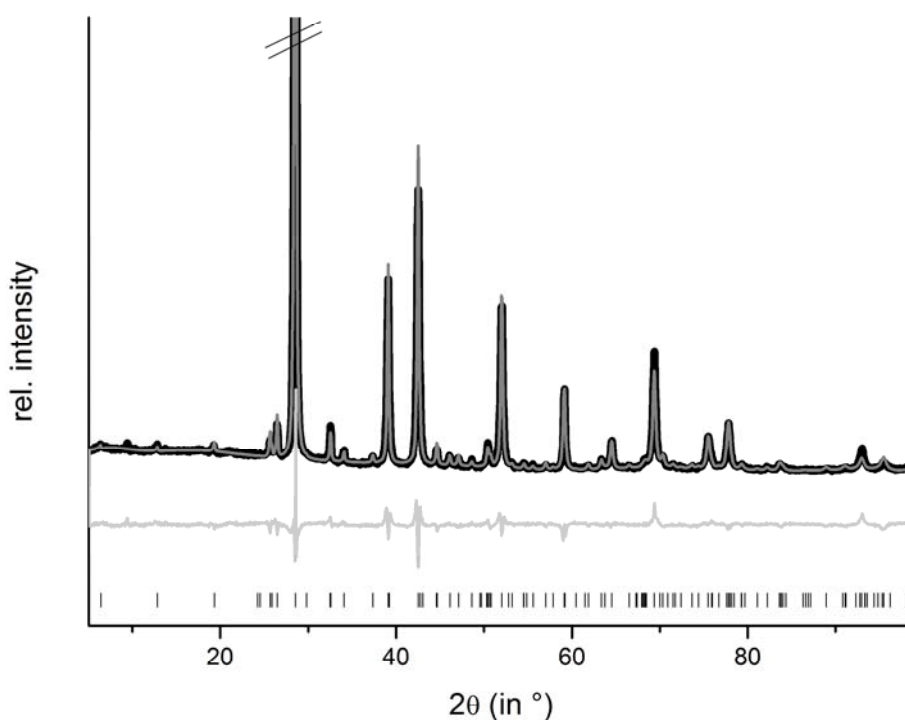


Figure S2: Rietveld refinement of $21R\text{-Ge}_{0.75}\text{Sn}_{0.25}\text{Sb}_2\text{Te}_4$ (the strongest reflection is cut off); vertical lines indicate calculated reflection positions, experimental (black) and calculated pattern (gray) and difference plot (below) are shown.

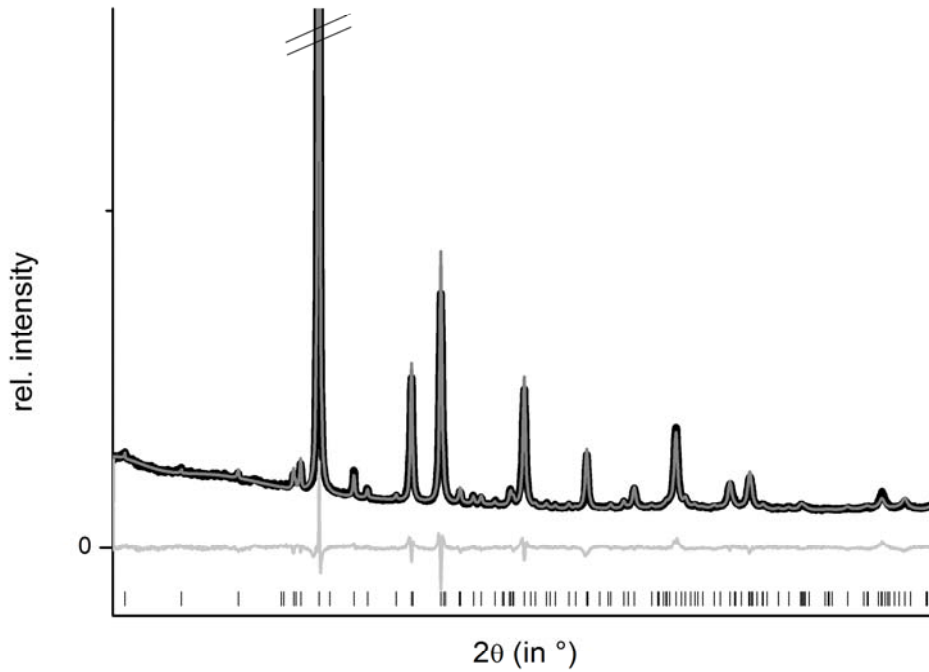


Figure S3: Rietveld refinement of 21R-Ge_{0.6}Sn_{0.4}Sb₂Te₄ (the strongest reflection is cut off); vertical lines indicate calculated reflection positions, experimental (black) and calculated pattern (gray) and difference plot (below) are shown.

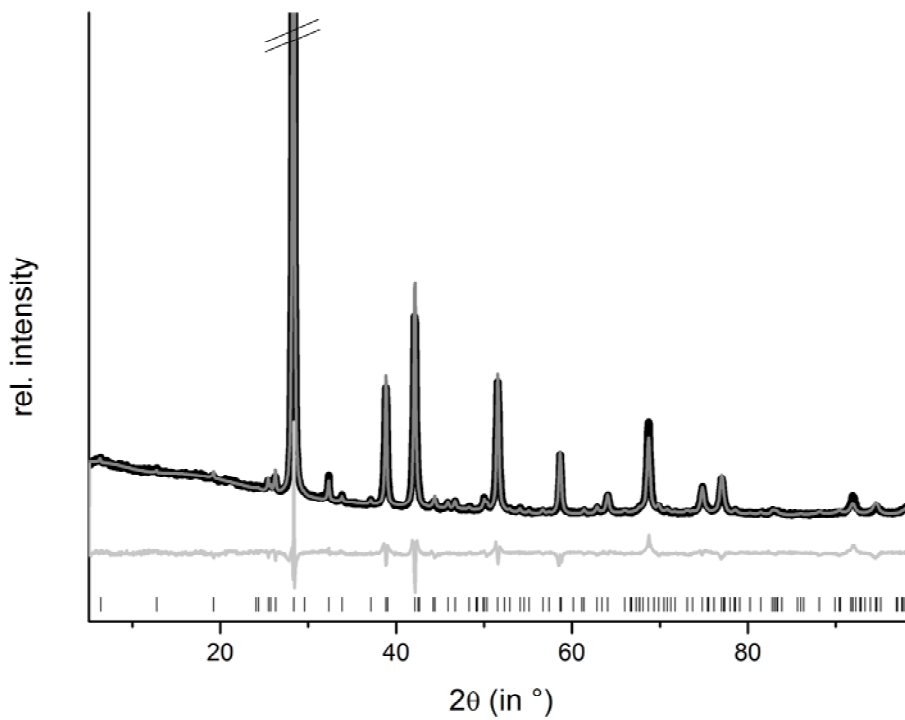


Figure S4: Rietveld refinement of 21R-Ge_{0.25}Sn_{0.75}Sb₂Te₄ (the strongest reflection is cut off); vertical lines indicate calculated reflection positions, experimental (black) and calculated pattern (gray) and difference plot (below) are shown.

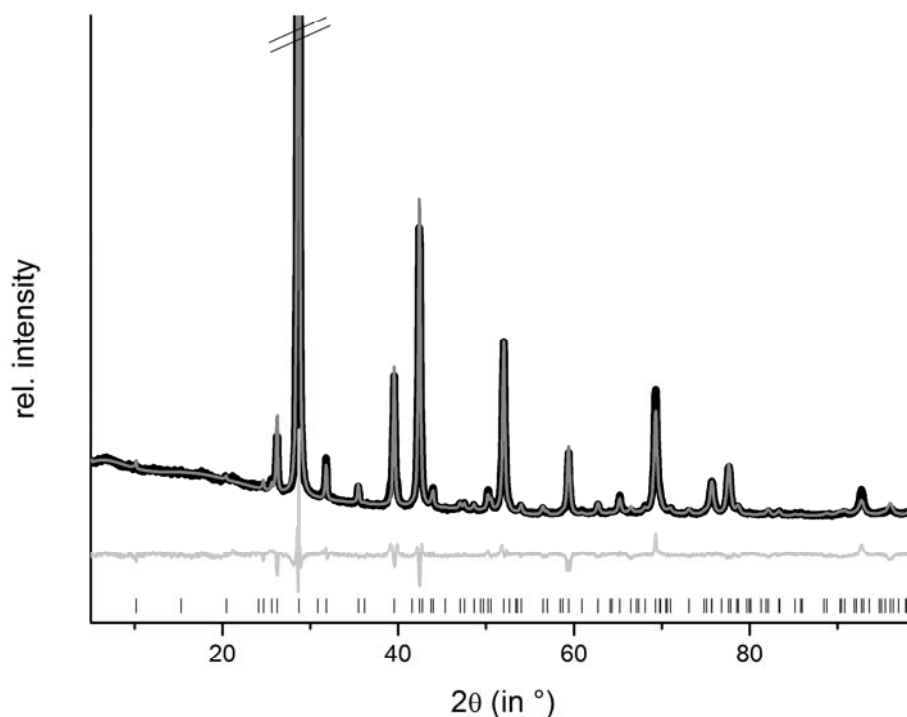


Figure S5: Rietveld refinement of $9P\text{-Ge}_{1.3}\text{Sn}_{0.7}\text{Sb}_2\text{Te}_5$; (the strongest reflection is cut off); vertical lines indicate calculated reflection positions, experimental (black) and calculated pattern (gray) and difference plot (below) are shown

Table S1: Specific annealing conditions of samples used for structure determination by Rietveld refinement; note that the exact temperatures and annealing times have little influence on the powder diffraction patterns and that many more samples with almost the same diffraction patterns were obtained at slightly different conditions.

Formula	Annealing time (in h)	Temperature (in °C)
$\text{Ge}_{0.75}\text{Sn}_{0.25}\text{Sb}_2\text{Te}_4$	46	560
$\text{Ge}_{0.6}\text{Sn}_{0.4}\text{Sb}_2\text{Te}_4$	144	540
$\text{Ge}_{0.5}\text{Sn}_{0.5}\text{Sb}_2\text{Te}_4$ *	20	550
$\text{Ge}_{0.25}\text{Sn}_{0.75}\text{Sb}_2\text{Te}_4$	46	560
$\text{Ge}_{1.3}\text{Sn}_{0.7}\text{Sb}_2\text{Te}_5$	46	490
$\text{GeSnSb}_2\text{Te}_5$	39	570

* The TEM-EDX measurements for $\text{Ge}_{0.5}\text{Sn}_{0.5}\text{Sb}_2\text{Te}_4$ were done with a sample that was annealed at 620 °C for 72 h and subsequently at 590 °C for 120 h.