



STRUCTURAL SCIENCE  
CRYSTAL ENGINEERING  
MATERIALS

Volume 75 (2019)

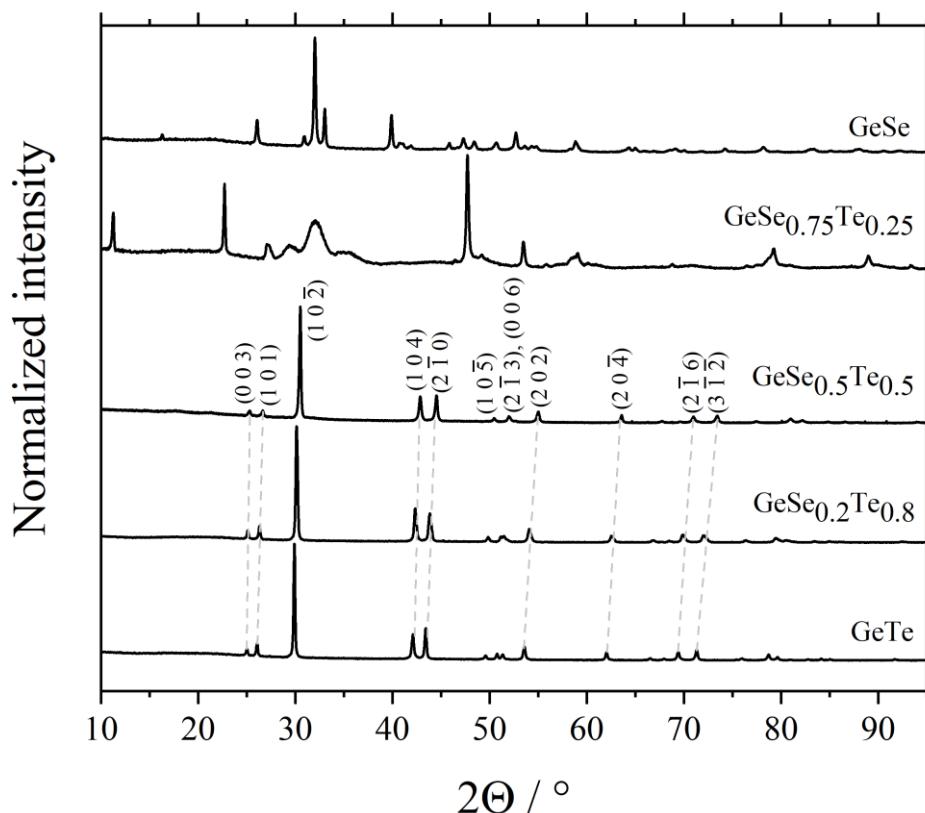
Supporting information for article:

New insights on the GeSexTe $1-x$  phase diagram from theory and experiment

Markus Guido Herrmann, Ralf Peter Stoffel, Michael Küpers, Mohammed Ait Haddouch, Andreas Eich, Andrzej Grzechnik, Richard Dronskowski and Karen Friese

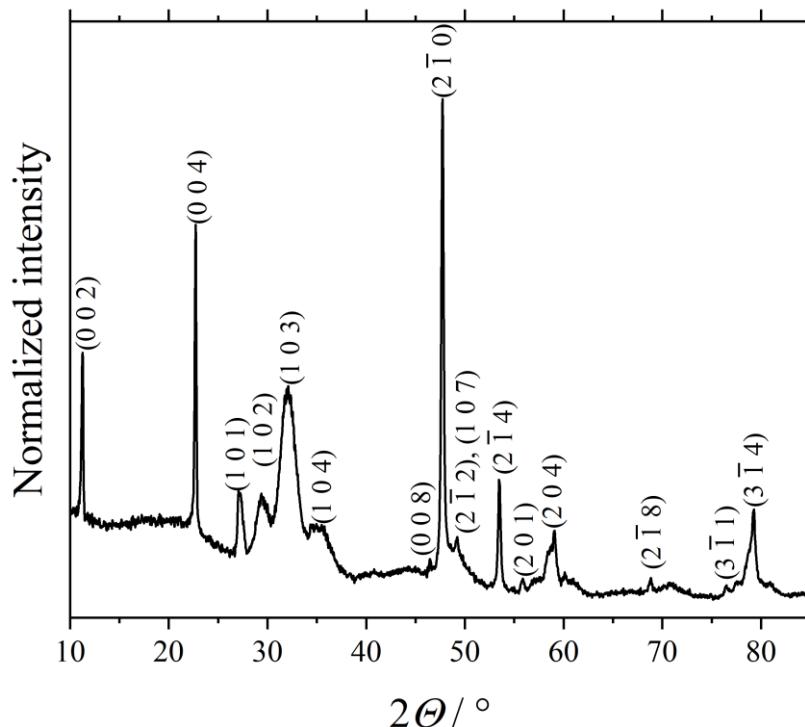
**S1. Indexed powder pattern****S1.1.  $\text{GeSe}_x\text{Te}_{1-x}$** 

Indexed powder pattern of the isostructural  $\text{GeSe}_x\text{Te}_{1-x}$  ( $x = 0, 0.2, 0.5$ ) mixed crystals between  $2\theta = 10\text{--}95^\circ$ . All peaks are indexed with the lattice parameter reported by Bauer Pereira [17]. Miller indices of parts of the peaks are indicated. The compositional shift of these peak is marked by grey dashed lines. For comparison the powder pattern collected for  $\text{Ge}_4\text{Se}_3\text{Te}$  and  $\text{GeSe}$  are also shown.



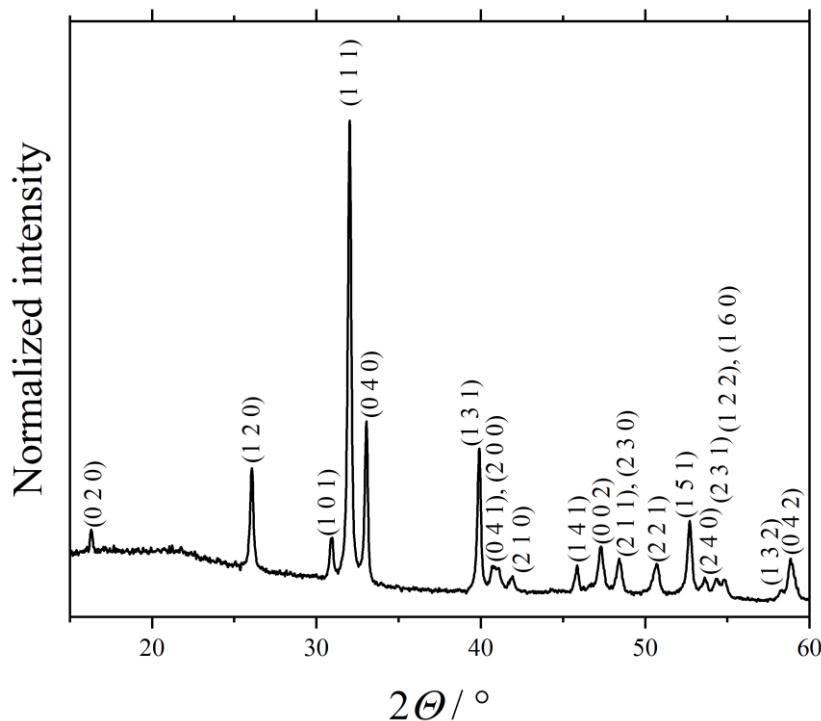
**S1.2. Ge<sub>4</sub>Se<sub>3</sub>Te**

Indexed powder pattern of Ge<sub>4</sub>Se<sub>3</sub>Te between  $2\theta = 10\text{--}85^\circ$ . All peaks are indexed with the lattice parameter reported by Küpers et al [13].



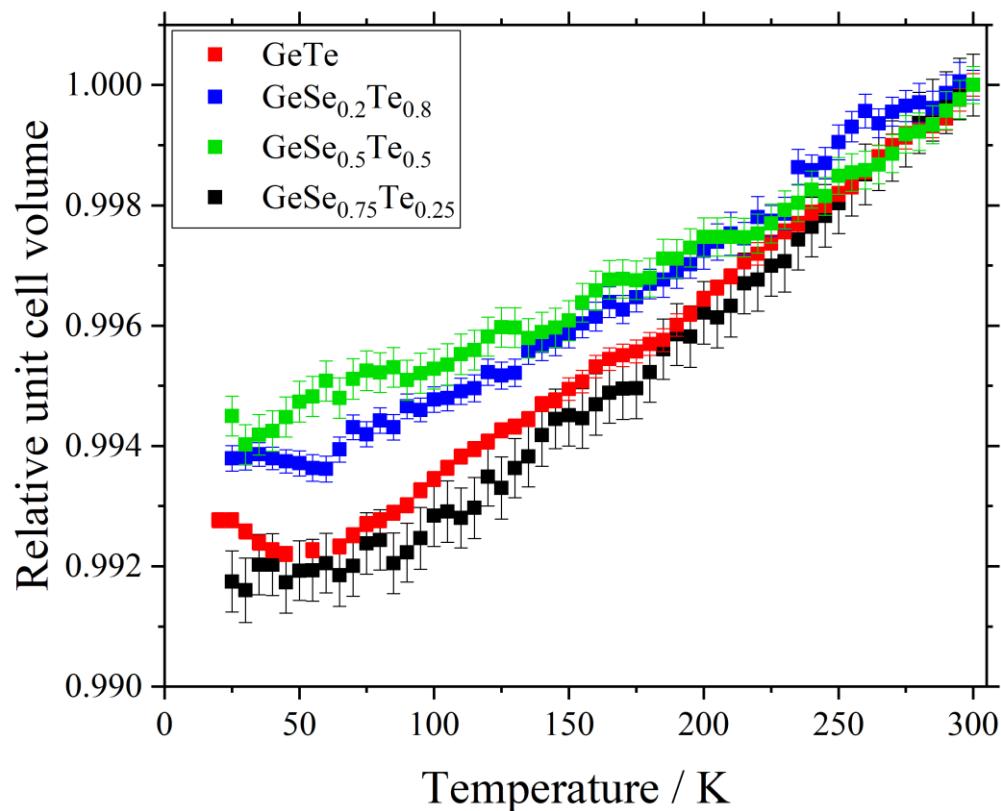
**S1.3. GeSe**

Indexed powder pattern of GeSe between  $2\theta = 10\text{--}60^\circ$ . All peaks are indexed with the lattice parameter reported by Wiedemeier et al [14].



**S2. Temperature dependence of the unit the volumes**

Temperature dependence of the normalized unit cell volumes of GeTe,  $\text{GeSe}_{0.2}\text{Te}_{0.8}$ ,  $\text{GeSe}_{0.5}\text{Te}_{0.5}$  and  $\text{Ge}_4\text{Se}_3\text{Te}$ .



### S3. Temperature dependence of the primitive lattice parameter

Lattice parameter of the corresponding primitive lattice of GeTe, GeSe<sub>0.2</sub>Te<sub>0.8</sub>, GeSe<sub>0.5</sub>Te<sub>0.5</sub> and Ge<sub>4</sub>Se<sub>3</sub>Te.

