

MS15-P09 | NEW INSIGHTS ON THE HIGH PRESSURE BEHAVIOUR OF THE $\text{GeSe}_x\text{Te}_{1-x}$ SOLID SOLUTION

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Binary chalcogenides of group IV–VI elements, e.g. GeTe, are candidates for optoelectronic and thermoelectric devices as well as for non-volatile phase-change memories. The incorporation of Se into GeTe has a positive influence on many of the desired properties [1]. At atmospheric conditions, GeTe-I is rhombohedral ($R3m$) [2]. Mixed crystals with $0 < x < 0.52$ are isostructural to GeTe-I, while a hexagonal phase was found for $0.58 < x < 0.85$ [2,3].

We performed synchrotron diffraction experiments and DFT calculations on $\text{GeSe}_x\text{Te}_{1-x}$ ($x=0, 0.2, 0.5, 0.75$) at high pressures. In particular, we studied the influence of Se on the stability fields of the phases and the effect of Ge...Ge interactions.

GeTe, $\text{GeSe}_{0.2}\text{Te}_{0.8}$, and $\text{GeSe}_{0.5}\text{Te}_{0.5}$ follow the transition pathway GeTe-I ($R3m$) \rightarrow GeTe-II (FCC) \rightarrow GeTe-III ($Pnma$) [4]. The structure of the GeTe-III polymorph was solved from single crystal data [4]. In the structure, which is different from earlier reported models, additional Ge...Ge and Se/Te...Se/Te interactions exist. GeTe-III is isostructural to beta-GeSe, a high-pressure and high-temperature polymorph of GeSe. The stabilization of GeTe-III is due to the strengthening of the longer Ge-Te bonds and of GeGe interactions.

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[2] Onodera A. et al., *Phys. Rev. B* **56**, 7635-41 (1997).

[3] Serebryanaya N.R. et al., *Phys. Lett. A* **197**, 63-66 (1995).

[4] Herrmann M.G. et al., *Acta Cryst. B* **75**, 246-256 (2019).