Rational Approaches to Synthesis and Crystal Growth of Rare Earth Metal Tellurides

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Binary Polychalcogenides LnX_x of trivalent rare earth metals (*Ln* = Y, La, Ce – Nd, Sm, Gd – Lu, *X* = S, Se, Te) exhibit a large structural variety. Within small compositional ranges originating from chalcogen defects, individual electronic situation leads to structural organization of different types of chalcogenide or polychalcogenide anions, accordingly, and thus very individual physical properties. For distinction of individual phases and for their detailed physical-chemical characterization, crystals of high quality are required.

Prior to experimental efforts a thermodynamic assessment of the binary systems *Ln*/Te is aspired in order to get a rational approach for suitable synthesis conditions. Here, the binary system Gd/Te serve as a model system for investigations of thermodynamic behavior of phase formation and for synthesis planning both in solid state reactions and crystal growth by vapor transport [1]. The evaluation of temperature and pressure dependent existence ranges of involved phases $GdTe_x$ started with modeling of the respective phase diagram (fig. 1a) using FactSage [2]. The experimental phase diagram Gd/Te is referenced to [3], and thermodynamic standard data were deduced from electrochemical measurements [4]. After optimization of standard data by fitting the experimental binary phase diagram further calculation of pressure dependent existence of binary phases has been realized concluding in the respective phase barogram (fig. 1b) [4]. For crystallization of $GdTe_x$ by chemical vapor transport [5] by using iodine as a mineralizer the ternary phase diagram Gd/Te/I has been assessed. Finally, reasonable vapor transport mechanism could be identified and crystal growth succeeded, fig. 1c.

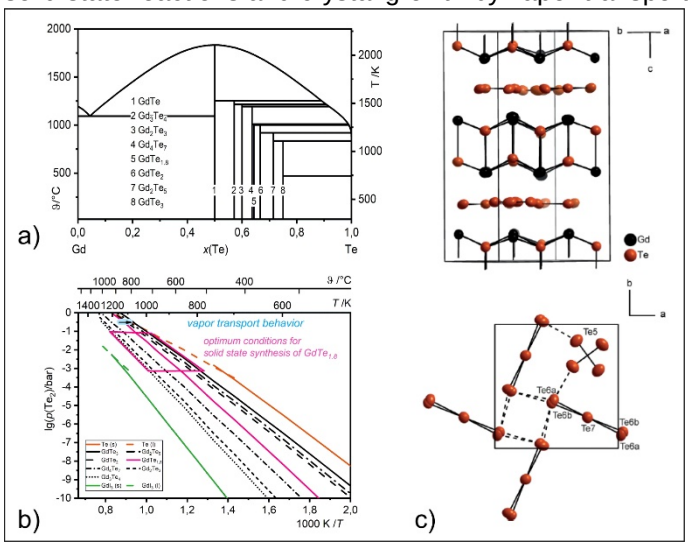

Figure 1. Thermodynamic assessment of the system Gd/Te and simulation of crystallization processes by vapor transport[1]: a) modelling of phase diagram, b) modelling of phase barogram, and c) visualization of crystal structure and arrangement of chalcogenide and polychalcogenide anions.

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