Thermodynamic analysis of the Sr-Se and Sr-Te systems using the calphad approach supported by ab initio calculations

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Abstract:

The II–VI compound semiconductors have recently received considerable interest from both experimental and theoretical points of view. This is due to their potential technological applications from the blue to the near ultraviolet spectral region. Among these compounds, the strontium chalcogenides SrX (X= Se and Te), together with other alkaline earth chalcogenides form a very important closed shell ionic system with NaCl crystal structure at normal conditions. In order to control the processing of such materials, an accurate knowledge of the phase diagram of those systems is required. In this work the assessment of the Sr-Se and Sr-Te systems, using a combined ab-initio and CALPHAD (CALculation of Phase Diagrams) approach, is presented.

The total energies of the equiatomic compounds SrSe and SrTe have been calculated by the full-potential linearized augmented plane wave (FLAPW) method with the generalized gradient approximation (GGA) using the WIEN2k software package. The thermodynamic assessments have been performed by using CALPHAD technique, based on the experimental data and calculated enthalpies of formation. The optimization was made using a computer program, which allows the simultaneous consideration of various types of thermodynamic data and phase diagram information. A set of self-consistent thermodynamic parameters for the Sr-Se and Sr-Te systems has been obtained, and the calculated results show a good agreement with the corresponding experimental data..

Contribution: Oral