

Étude des propriétés structurales électroniques et thermodynamiques de l'alliage quaternaire $\text{Zn}_{1-x}\text{Mg}_x\text{Se}_y\text{Te}_{1-y}$

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Abstract: First-principles calculations are performed to study the structural, electronic and thermodynamic properties of $\text{Zn}_{1-x}\text{Mg}_x\text{Se}_y\text{Te}_{1-y}$ alloys using the full potential-linearized augmented plane wave method (FP-LAPW) within the density functional theory (DFT). In this approach the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA) was used for the exchange-correlation potential. Moreover, the modified Becke Johnson approximation (mBJ) was also used for band structure calculations. First for the MgX binary compounds various phases were considered in order to confirm the most stable one and to predict the transition pressure between different phases. The lattice constant for the ternary alloys exhibits a small deviation from the Vegard's law. The microscopic origins of the gap bowing were explained by using the approach of Zunger and co-workers. The bowing of the fundamental gap versus composition predicted by our calculations is in good agreement with available theoretical data. In addition, we have studied the thermal properties of these alloys using the Debye model implemented in Gibbs program. Finally, the energy band gap of $\text{Zn}_{1-x}\text{Mg}_x\text{Se}_y\text{Te}_{1-y}$ quaternary alloys lattice matched to InAs and ZnTe substrates was investigated. To our knowledge this is the first quantitative theoretical investigation on $\text{Zn}_{1-x}\text{Mg}_x\text{Se}_y\text{Te}_{1-y}$ quaternary alloys and still awaits experimental confirmations.

Keywords : $\text{Zn}_{1-x}\text{Mg}_x\text{Se}_y\text{Te}_{1-y}$ Quaternary alloys, Functional density (DFT), Approximation of the generalized gradient (PBE-GGA), mBJ approximation, InAs and ZnTe substrates