Étude des propriétés structurales électroniques et thermodynamiques de l'alliage quaternaireZn1-xMgxSeyTe1-y

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Abstract: First-principles calculations are performed to study the structural, electronic and thermodynamic properties of Zn1-xMgxSeyTe1-yalloys using the full potential-linearized augmented plane wave method (FP-LAPW) within the density functional theory (DFT). In this approach the Perdew-Burke-Ernzerhorf 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 compoundsvarious phases were considered in order to confirm the most stable one and to predict the transition pressure between different phases. The lattice constant for theternary 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 Zn1-xMgxSeyTe1-y quaternary alloys lattice matched to InAsandZnTesubstrats was investigated. To our knowledge this is the first quantitative theoretical investigation on Zn1-xMgxSeyTe1-y quaternary alloys and still awaits experimental confirmations.

Keywords : Zn1-xMgxSeyTe1-y Quaternary alloys, Functional density (DFT), Approximation of the generalized gradient (PBE-GGA), mBJ approximation, InAs and ZnTe substrates