World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

High-Pressure Calculations of the Elastic Properties of ZnSx Se 1−x Alloy in the Virtual-Crystal Approximation

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Abstract : We report first-principles calculation results on the structural and elastic properties of ZnS x Se1−x alloy for which we employed the virtual crystal approximation provided with the ABINIT program. The calculations done using density functional theory within the local density approximation and employing the virtual-crystal approximation, we made a comparative study between the numerical results obtained from ab-initio calculation using ABINIT or Wien2k within the Density Functional Theory framework with either Local Density Approximation or Generalized Gradient approximation and the pseudo-potential plane-wave method with the Hartwigzen Goedecker Hutter scheme potentials. It is found that the lattice parameter, the phase transition pressure, and the elastic constants (and their derivative with respect to the pressure) follow a quadratic law in x. The variation of the elastic constants is also numerically studied and the phase transformations are discussed in relation to the mechanical stability criteria.

Keywords : density functional theory, elastic properties, ZnS, ZnSe,
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020