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Molecular Dynamics Simulations of the Structural, Elastic and Thermodynamic Properties of Cubic GaBi

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Abstract : We present the molecular dynamic simulations results of the structural and dynamical properties of the zinc-blende GaBi over a wide range of temperature (300-1000) K. Our simulation where performed in the framework of the three-body Tersoff potential, which accurately reproduces the lattice constants and elastic constants of the GaBi. A good agreement was found between our calculated results and the available theoretical data of the lattice constant, the bulk modulus and the cohesive energy. Our study allows us to predict the thermodynamic properties such as the specific heat and the lattice thermal expansion. In addition, this method allows us to check its ability to predict the phase transition of this compound. In particular, the transition pressure to the rock-salt phase is calculated and the results are compared with other available works.

Keywords : Gallium compounds, molecular dynamics simulations, interatomic potential thermodynamic properties, structural phase transition
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