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

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Abstract : We present a theoretical study of the structural, elastic and thermodynamic properties of the zinc-blende AlBi for a wide temperature range. The simulation calculation is performed in the framework of the molecular dynamics method using the three-body Tersoff potential which reproduces provide, with reasonable accuracy, the lattice constants and elastic constants. Our results for the lattice constant, the bulk modulus and cohesive energy are in good agreement with other theoretical available works. Other thermodynamic properties such as the specific heat and the lattice thermal expansion can also be predicted. 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 : aluminium compounds, molecular dynamics simulations, interatomic potential, thermodynamic properties, structural phase transition
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