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Pressure Induced Phase Transition of Semiconducting Alloy TlxGa1-xAs

Authors : Madhu Sarwan, Ritu Dubey, Sadhna Singh

Abstract : We have investigated the structural phase transition from Zinc-Blende (ZB) to Rock-Salt (RS) structure of TlxGa1-xAs by using Interaction Potential Model (IPM). The IPM consists of Coulomb interaction, Three-Body Interaction (TBI), Van Der Wall (vdW) interaction and overlap repulsive short range interaction. The structural phase transition has been computed by using the vegard's law. The volume collapse is also computed for this alloy. We have also investigated the second order elastic constants with composition for the alloy TlxGa1-xAs.

Keywords : III-V alloy, elastic moduli, phase transition, semiconductors
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