Molecular Dynamics Simulations of Indium Antimonite Under High Pressure

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Abstract – Using Molecular Dynamics Simulations (MD) the energetic sequence of structures of Indium Antimonite (InSb) is calculated. MD is performed to study high pressure phases of InSb up to 70 GPa. The structural phase transformation induced by increasing pressure drives a Zinc Blend (ZB) to Rock-Salt (RS) structural transition and from Rock-Salt to Cesium Chloride (CC) expected to occur at high pressures. The effective empirical interatomic potential proposed consists of two and three body interactions which has the same functional form of the interatomic potential proposed by Vashishta et. al. [1-4] to study other semiconductors.

Large scale simulations, requiring several million of atoms or long times, has been possible with the use of good empirical interatomic potential. These empirical potentials express the total energy of the system of atoms as a function of its atomic positions. The energy for InSb is modeled as a sum of two and three body interactions. The pair potential includes Coulomb, steric repulsion, charge-dipole and dipole-dipole interactions. The three body interactions consider bond bend and bond stretching. A potential energy function attained for InSb is flexible and accommodates as wide a range as possible of fitting data. This data include crystalline lattice constants, the stability of the structures as well as the other structural transformation at high pressures, cohesive energies, elastic properties and Vibrational Density of States. The accuracy of the potential is guaranteed reproducing these properties in accord with experimental results. The most important feature of a good empirical potential is not only it accuracy but also its transferability.[5]

All simulations reported here were done in NPT ensemble with systems containing 1000, 10648, and 110512 particles. The equations of motion were integrated using velocity Verlet algorithm with a time step of 1.5fs.

In addition, the structures attained with different pressure, not included in a fitting data base, are correctly reproduced. The static and dynamic dependence with pressure was obtained. Starting with a zinc blend phase at fixed temperature, the external pressure was increased in steps of few MPa every 2000 time steps, up to 70 GPa. The ZB structure is dynamically stable up to 3.0GPa, and the agreement with experimental result of Vanderborgh et al.[6] is very good.

A further increase in hydrostatic pressure causes new first order phase transformation at 49GPa. Structural characterization using two and three body correlations indicates that this new phase has features of a cesium chloride structure. The CsCl phase is stable up to 70GPa (the maximum simulated pressure) and the backward transformation occurs with a large hysteresis, back transforming to RS at 20 GPa. Further reduction in pressure shows that the RS phase is stable up to 0GPa. It has been conjectured that the CsCl should be the natural high pressure phase, but as far as we know it has never been confirmed experimentally [7]. Further validation of the model was obtained by calculating the vibrational density of states and compare with the deformable-bond approximation (DBA) [8,9] which is based on the experimental phonon dispersion relation reported by Price et al. [10]. The results are in good agreement with the calculated density of states. Once the results from the simulation reproduce very well these quantities, all parameters in the interatomic potential are kept constant to simulate other properties. In summary, at zero pressure the vibrational density of states is correctly described and when applying hydrostatic pressure two first order transitions were observed: ZB to RS and to CsCl structures. The transition and the equation of state were correctly obtained, in very good agreement with experiments.

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