Abstract Submitted
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Germanium under Shock Waves: A Study of Some Physical Properties by First Principles Method ENAMUL HAQUE, None, M. D. I. BHUYAN COLLABORATION — We have explored some physical properties of germanium under shock waves, such as elasticity and compressibility, with first principles method, conductivity, susceptibility, and heat absorbability in Comsol environment. The equations of state used for investigation of the above properties relating phase transitions between crystal structures are based on ab initio predictions of the electron in ground states. The deduced equations of state have matched in reasonable range with data on the shock Hugoniot and the calculated physical parameters have coincided in reasonable error with the available value. However, electromagnetic properties of germanium have varied significantly under shock waves, with applied pressure 5GPa. The variation of band energy with pressure has been calculated. The elastic properties have also verified with density functional theory (DFT) which shows excellent accuracy of the result. The possible explanation of these physical properties of germanium is briefly described.

Enamul Haque
None

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