ANISOTROPY AND PRESSURE EFFECT ON THE ELASTIC AND MECHANICAL PROPERTIES OF (B3) BN

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S u m m a r y

We present the results of *ab initio* calculations of the anisotropy and hydrostatic pressure effects on the elastic and mechanical properties of (B3) boron nitride, using the density functional perturbation theory (DFPT). The independent elastic and compliance constants, bulk and shear moduli, Zener anisotropy and Kleinman parameters, Cauchy and Born coefficients, Young modulus, and Poisson's ratio for directions within the important crystallographic planes of this compound under pressure are obtained. The crystal density, the longitudinal, transverse, and average sound velocities, and the Debye temperature under pressure are also studied. In the investigation of the stability criteria, the results showed a phase transition pressure from zinc blende to the rock-salt phase at about 4.54 Mbar, which is in good agreement with some available theoretical data reported in the literature and shows discrepancies with another ones.