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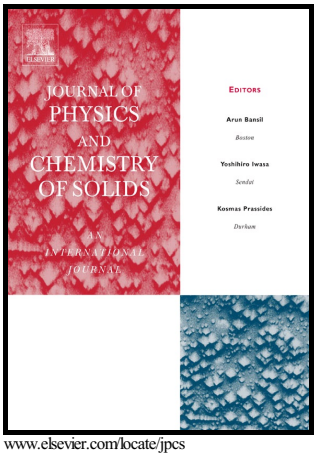

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Pressure effect on the mechanical, electronic and thermodynamic properties of Ba_2Bi_3: first-principle calculations

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Abstract

The newly discovered Ba_2Bi_3 phase has attracted attentions in search of new superconductors, mainly because of the layered structure with two-dimensional superconducting Bi planes intercalated by Ba atoms. To clearly reveal what features the layered structure of the Ba_2Bi_3 phase correlates with, especially under pressure, we have systematically investigated the structural, mechanical, electronic and thermodynamic properties under the equivalent hydrostatic pressures up to 14 GPa by means of first-principle calculations with the Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) approaches. The results indicate that the pressure effect on the crystal structure is performed as a compression of the unit-cell volume, mainly along the c-axis. Specifically for the mechanical related properties, the elastic constants and polycrystalline elastic moduli monotonically increase with the pressure. The calculated ductile factors show that the Ba_2Bi_3 lies in between the brittle and ductile border line at 0 GPa and the pressure makes the ductility enhancement. Besides, the anisotropic properties of the Ba_2Bi_3 under various pressures are discussed. The electronic energy band structure and density of states under pressure are analyzed. Moreover, the pressure and temperature dependence of the thermodynamic properties through the quasi-harmonic Debye model, together with the pressure dependence of the Debye temperature calculated from elastic constants has been obtained. The calculated results of the variation of the Debye temperature and total density of states at Fermi level show that the pressure can lead to the superconducting transition temperature (T_c) of the Ba_2Bi_3 decreasing.

Keywords

Ba_2Bi_3 superconductor; Mechanical properties; Electronic properties; Thermodynamic properties; First-principle calculations.