Indian J Phys (September 2022) 96(11):3191–3200
https://doi.org/10.1007/s12648-021-02278-9

ORIGINAL PAPER

Elastic, mechanical and ultrasonic studies of boron monopnictides in two different structural phases

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Received: 05 July 2021 / Accepted: 24 December 2021 / Published online: 9 February 2022

Abstract: In the present study, elastic, mechanical, thermo-physical and ultrasonic properties of boron monopnictides BX (X = N, P, As) in both NaCl (B1) and CsCl (B2) phases have been investigated at room temperature. Coulomb and Born–Mayer potential model has been used for the calculation of second- and third-order elastic constants (SOECs and TOECs) of BX in both B1 and B2 phases. The calculated values of SOECs have been applied for the evaluation of the mechanical properties of these compounds using Voigt–Reuss–Hill approximation. The Born stability criteria and Vicker's hardness parameter (H) have been used for the analysis of nature and strength of the chosen materials. Later on, ultrasonic velocities including Debye average velocities have been evaluated utilizing calculated values of SOECs and density of the chosen materials. Thermal properties of the materials such as the lattice thermal conductivity, thermal relaxation time, thermal energy density and acoustic coupling constant have been also computed along $< 100 >$ direction. These computed thermo-physical properties indicate that BP and BAs show metallic behaviour in B1 phase, while BN shows a metallic behaviour in both phases. Finally, ultrasonic attenuation has been estimated for these materials at room temperature along $< 100 >$ direction. The obtained results have been compared with available results and discussed with available findings on these types of materials.

Keywords: Elastic constants; Mechanical property; Thermophysical property; Ultrasonic attenuation

1. Introduction

In the past few years, boron compounds have gained huge interest due to their wide industrial applications [1]. The boron is similar to carbon, having one electron less compared to the latter. When boron is combined with metal atoms, it leads to acquiring stable structured and forms metal-boron cluster compounds, especially with rare earth elements, which are localized with 4f orbitals. The boron is inherently p electron-deficient and has a small core size that causes B-doped molecules to have unique physical properties. Nowadays, these compounds are widely used in electronic, optical and medical fields [2, 3]. For instance, boron-based materials are used to enhance the photophysical properties of compounds, which are making them useful in luminescent and sensor materials. In particular, boron monopnictides with P and As were predicted to improve the thermal conductivity. Among these, boron monopnictides BX (X: N, P, As) are of particular interest for being B as anion and other as the most covalent one which in turn helps to advance the properties of materials. Most of the boron-based compounds possess outstanding physical properties such as high Pugh's indicator, ductility, hardness and thermal conductivity [4–6]. While few of them have attained other properties which include low density, low attenuation and higher resistivity [7, 8].

Various techniques and approaches were used to estimate the physical properties of boron-based compounds in different ambience conditions like pressure, temperature, phase of structure [9, 10]. Some important elastic, thermal and anisotropic properties of boron-based compounds (BP and BAs) were studied and elaborated by Dong et al. [11]

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