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ELASTIC CONSTANTS AND ITS PRESSURE DERIVATIVE OF BORON PHOSPHIDE USING HIGHER-ORDER PERTURBATION THEORY

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The elastic constants, pressure derivative of bulk modulus and pressure derivative of elastic constants are investigated using the higher-order perturbation theory based on pseudopotential formalism and the application of our proposed model potential for Boron Phosphide. The parameter of the potential is derived using zero-pressure equilibrium condition. In the present study, Hartree and Sarkar et al screening functions are used to consider exchange and correlation effect. The good agreement of presently investigated numerical data is found with the available experiment data and other such theoretical values.

Keywords: *PSEUDOPOTENTIAL METHOD, ELASTIC CONSTANTS, PRESSURE DERIVATIVE OF ELASTIC CONSTANTS.*

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1. INTRODUCTION

Boron compounds have unique physical properties such as low densities, extremely high thermal conductivities, wide band-gap and large resistivities etc. and hence these materials are of great technological interest for high-temperature, electronic and optical applications. Due to such technological importance of these materials it is essential to understand various physical properties of such semiconductor compound and hence the study of properties of these semiconductors has attracted the interest of researcher for last few years [1-6].

Previously, we have successfully used higher-order perturbation theory to calculate many physical properties of Group IV, Group III-V and II-VI elemental and compound semiconductors using model potential proposed by Jivani et al. [7-10]. In the present paper, we have applied Jivani et al model potential [7-10] for the investigation of elastic constants and its pressure derivative for BP in zinc-blende phase.

2. METHOD OF COMPUTATIONS

For a crystal with zinc-blende structure based on the higher-order perturbation theory, the total energy per electron of the crystal [7-10] is given by

$$E = E_{\mathrm{i}} + E_0 + E_1 + E_2 + E_{cov}. \qquad (1)$$

In equation (1), E_i is electrostatic energy of point ions immersed in the uniform gas of valence electrons, E_0 is the sum of the kinetic, exchange and correlation energies of the valence electron, E_1 and E_2 are the first and second-order perturbation energy and E_{cov} is covalent correction term.

In the present work, the model potential proposed by Jivani et al. [7-10] in momentum-space is employed which is given by

$$W_b(q) = -\frac{12\ \pi\ Z e^2}{\Omega q^3\ \ R_C}\left[\frac{\sin(qR_C)}{2} - \frac{1}{q\ R_C} + \frac{\sin(qR_C)}{(qR_C)^2}\right]. \qquad (2)$$

Here Ω is the atomic volume, q is wave vector, Z is ion valency, e is the electronic charge and R_C is the parameter of the potential. The value of parameter is determined by using zero pressure equilibrium condition. For the incorporation of exchange and correlation effects to the dielectric function, we adopted two considerations, Hartree (H) [11] and Sarkar et al. (S) [12].

3. RESULTS AND DISCUSSION

3.1 The elastic constants

The elastic constants (C_{11}, C_{12} and C_{44}) resulting from higher-order perturbation theory and homogeneous deformation method are summarized in Table 1 for BP. The values of presently investigated elastic constants are varying with the use of different local-field correction functions. There is a large variation in the other theoretical reported values [1-7] of the elastic constants (C_{11}, C_{12} and C_{44}) as observed from the Table 1. This is due to different approach used in the particular study. From the present outcome, we can conclude that the results were qualitatively in good agreement with the observed data and available other theoretical reported values.

Table 1 *– The elastic constants (C_{11}, C_{12} and C_{44} in GPa) for BP.*

Elastic Constants	With different f(q)		Expt. [13]	Other [1-7]
	H [11]	S [12]		
C_{11}	316.93	311.03	315	329, 337, 357, 359, 360
C_{12}	60.831	103.98	100	78, 81, 87, 97.5, 155
C_{44}	114.28	117.01	160	146, 150, 154, 175, 200, 202

3.2 Pressure derivatives of bulk modulus and elastic constants

In Table 2, the presently investigated pressure derivative of bulk modulus and elastic constants and the pressure derivatives of the elastic constants for BP are displayed along with other such theoretical results [1-7] as well as experimental data [14]. Our investigated result of the pressure derivative of bulk modulus is comparable with the results due to other theoretical methods [1-7]. As per our knowledge, the pressure derivative of elastic constants for BP are not reported so far and hence present results may be useful to compare with the future experimental and theoretical investigations.

Table 2 – *Pressure derivatives of bulk modulus and elastic constants for BP*

C'_i	With different f(q)		Experimental [14]	Other [1-7]
	H[11]	S [12]		
B'	4.77	3.97	4.3 ± 0.5	3.07, 3.58, 3.68, 3.7, 3.712, 3.76, 3.92, 4.02, 4.3
C'_{11}	6.42	5.03	-	-
C'_{12}	3.94	3.44	-	-
C'_{44}	1.38	0.93	-	-

4. CONCLUSIONS

Finally, we conclude from the present study that presently investigated elastic constants and pressure derivative of bulk modulus and pressure derivative of elastic constants for boron phosphide agree well with the available experimental results and other theoretical calculations. Present study also shows that the effect of screening plays an important role in the investigations of such physical properties. The present numerical data may be useful for comparison purpose in future for theoretical as well as experimental study.

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