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# Insight into the unusual electronic structure of III-V boron compounds

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## Abstract

*We review the fundamental electronic structure of zinc-blende boron compounds BP, BAs, BSb, and BBi in the light of experimental and theoretical works. The resulting electronic, structural, bonding, pressure, alloying and dynamical properties are discussed.*

## Introduction

Recent experimental [1-5] and theoretical [6-15] studies have revived the interest to details of the

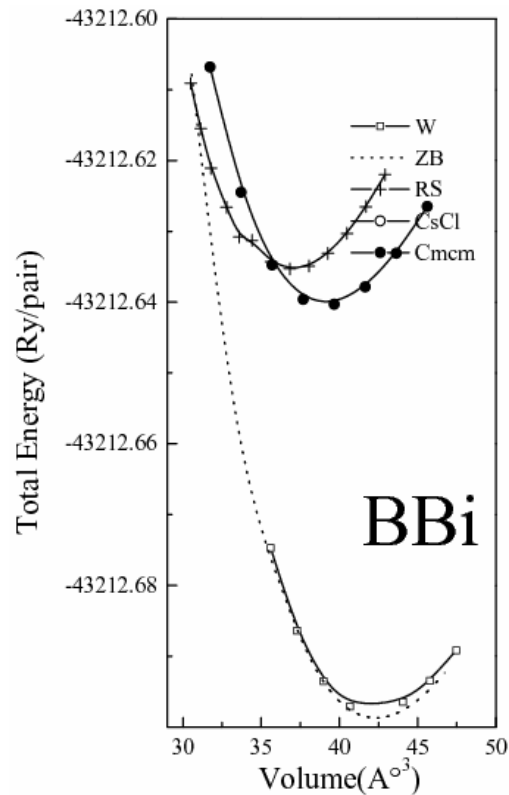
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electronic structure of III-V boron compounds. This interest stems from the fact of great technological interest for high temperature, electronic and optical applications. These compounds also are the candidates for applications in multi-junction solar cells and detectors. They possess unusual electronic properties relative to the more conventional zinc-blende III-V compounds. One reason is related to their extreme properties such low ionicity [16-19], short bond lengths [20], high mechanical strength [6,20] and elastic moduli [6,21], high melting point [22], wide [23] or even negative [9,24] band gap and strong optical band gap bowing [15].

The compounds considered here are BP, BAs, BSb and BBi (we don't consider BN, because it behaves much more like nitride materials than boride ones). From the basic point of electronic structure, the chief distinction of B-V semiconductors is: (a) the competition between the strong attractive B potential with the element V's potential for electronic and bonding properties, (b) strong disparity in atomic sizes between boron and other atoms of column V creating peculiar behaviour not seen in other compounds of the III-V family.

In this contribution, the electronic structure of III-V boron compounds is reviewed.



**Figure 1.** Total energy versus volume for the zinc-blende (ZB), wurtzite (W), rocksalt (RS), CsCl-type, and Cmcm phases of BBi.

## Structural properties

The III-V boron compounds crystallize in the zinc-blende phase as shown theoretically and experimentally for BP, BAs, and BSb. However, BBi which is the last member of this series has not been synthesized yet and it has been the subject of a few recent theoretical works [9,24,25] reporting that the zinc-blend phase is the ground state of BBi (Figure 1) as for the others borides. Theoretical calculations show that wurtzite (W) and zinc-blende (ZB) phases present very weak total energy difference [21,24,25], but the ZB phase is preferred over the W phase for the boron-V considered here (see Table 1).

The structural parameters and elastic constants for boron compounds are given in Table 1. These compounds have small lattice constants, significant bulk moduli, and elastic constants compared with the other III-V compounds.

**Table 1.** Structural parameters, elastic constants, and difference of total energy between wurtzite and zinc-blende phases ( $\Delta E_{W-ZB}$ ) for boron compounds.

		$a$ , Å	$B$ , GPa	$C_{11}$ , GPa	$C_{12}$ , GPa	$C_{44}$ , GPa	$\Delta E_{W-ZB}$ , meV
<b>BP</b>	Exp.	4.538 <sup>a</sup>	173 <sup>b</sup>	315 <sup>b</sup>	100 <sup>b</sup>	160 <sup>b</sup>	
	Cal.	4.558 <sup>c</sup> 4.554 <sup>d</sup>	160 <sup>d</sup>	337 <sup>d</sup> 359 <sup>e</sup>	78 <sup>d</sup> 80.6 <sup>e</sup>	200 <sup>d</sup> 196.7 <sup>e</sup>	20 <sup>e</sup>
<b>BAs</b>	Exp.	4.777 <sup>a</sup>	148 <sup>f</sup>				
	Cal.	4.777 <sup>c</sup> 4.812 <sup>d</sup>	133 <sup>d</sup>	275 <sup>d</sup> 291 <sup>e</sup>	63 <sup>d</sup> 72.8 <sup>e</sup>	150 <sup>d</sup> 157.9 <sup>e</sup>	15.76 <sup>e</sup>
<b>BSb</b>	Exp.						
	Cal.	5.12 <sup>g</sup> 5.278 <sup>d</sup>	115 <sup>g</sup> 100 <sup>d</sup>	207 <sup>d</sup> 205 <sup>e</sup>	47 <sup>d</sup> 62.5 <sup>e</sup>	105 <sup>d</sup> 121.1 <sup>e</sup>	6.74 <sup>e</sup>
<b>BBi</b>	Exp.						
	Cal.	5.416 <sup>h</sup> 5.39 <sup>i</sup>	86.27 <sup>h</sup>	163.8 <sup>h</sup> 160.2 <sup>e</sup>	28.3 <sup>h</sup> 51.5 <sup>e</sup>	86.3 <sup>h</sup> 87.4 <sup>e</sup>	15.56 <sup>e</sup>

<sup>a</sup> [26], <sup>b</sup> [27], <sup>c</sup> [20], <sup>d</sup> [6], <sup>e</sup> [21], <sup>f</sup> [28], <sup>g</sup> [29], <sup>h</sup> [24], <sup>i</sup> [30].

## Electronic properties

There are a limited experimental data regarding the electronic structure of these compounds. Experimentally for BP and BAs, minimum band gap is

found near X point, while no data exist for BBi and BSb. The most accurate calculations to date for boron compounds are the ab initio GW-pseudopotentials calculations of Surh et al [23] for BP and BAs, which qualitative agreement is found with experimental results. The important features of the band structure of BP, BAs, BSb and BBi are given in Table 2.

**Table 2.** Band gap energies (eV) of boron compounds.

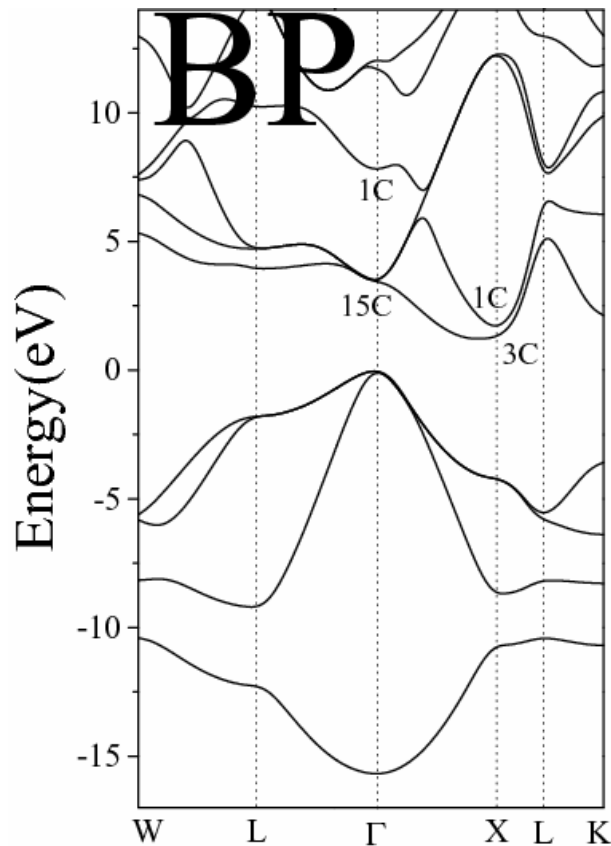
	Theo.	Exp.
<b>BP</b>	GW	
$\Gamma_{15v} \rightarrow \Delta_{\min}$	1.9 <sup>a</sup>	2.02 <sup>b</sup>
$\Gamma_{15v} \rightarrow \Gamma_{15c}$	4.4 <sup>a</sup>	5.0 <sup>c</sup>
$\Gamma_{15v} \rightarrow \Gamma_{1c}$	8.4 <sup>a</sup>	
<b>BAs</b>	GW	
$\Gamma_{15v} \rightarrow \Delta_{\min}$	1.6 <sup>a</sup>	0.67 <sup>d</sup>
$\Gamma_{15v} \rightarrow \Gamma_{15c}$	4.2 <sup>a</sup>	1.46 <sup>d</sup>
$\Gamma_{15v} \rightarrow \Gamma_{1c}$	5.5 <sup>a</sup>	
<b>BSb</b>	LDA	
$\Gamma_{15v} \rightarrow \Delta_{\min}$	0.52 <sup>e</sup>	
$\Gamma_{15v} \rightarrow \Gamma_{15c}$	3.06 <sup>e</sup>	
$\Gamma_{15v} \rightarrow \Gamma_{1c}$	3.28 <sup>e</sup>	
<b>BBi</b>	GGA	
$\Gamma_{15v} \rightarrow \Gamma_{6c}$	0.0858 <sup>f</sup>	
$\Gamma_{15v} \rightarrow \Delta_{\min}$	0.5 <sup>f</sup>	
$\Gamma_{15v} \rightarrow L_{6c}$	0.1 <sup>f</sup>	

<sup>a</sup> [23], <sup>b</sup> [31], <sup>c</sup> [32], <sup>d</sup> [33], <sup>e</sup> [29], <sup>f</sup> [24].

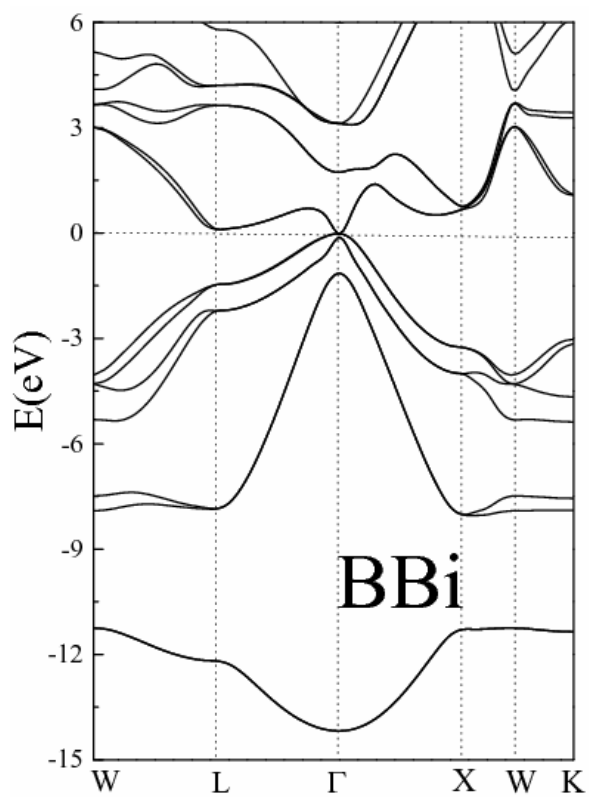
In Figure 2 we present the band structure of BP as prototype of boron family. The most prominent features of the band structure are:

- the minimum gap is found close to X point ( $\Delta_{\min}$  is close to X) as found for BAs and BSb, but not for BBi (see Figure 3);
- the lowest conduction band at X point is  $X_{3c}$  instead of  $X_{1c}$  as was found in most III-V semiconductors.  $X_{3c}$  ( $X_{1c}$ ) is a typical antibonding state with charge density mostly concentrated in the interstitial region close to the anion (cation) (see Figure 4);

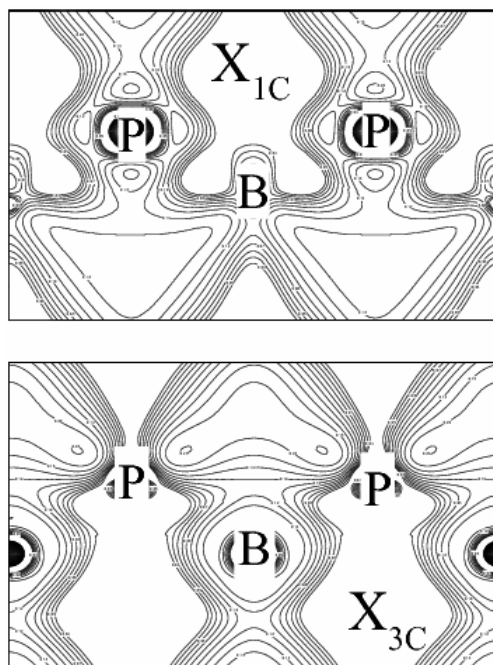
- (c)  $\Gamma_{15c}$  band is below the  $\Gamma_{1c}$  band, in contrast to other III-V compounds where the  $\Gamma_{1c}$  state is below the  $\Gamma_{15c}$  state. The boron compounds are characterized by a strong level repulsion (*s-s* interaction) [18] between  $\Gamma_{1v}$  and  $\Gamma_{1c}$ . As a consequence, the cation and anion *s* levels strongly interact and push  $\Gamma_{1c}$  above  $\Gamma_{15c}$ ;
- (d) small splitting at X point ( $X_{3v}-X_{1v}$ ) compared with III-V compounds. For instance, splitting increases (decreases) with increasing (decreasing) electronegativity mismatch inducing a weak ionicity of boron compounds compared with other III-V compounds;
- (e) strong *p-p* mixing in the valence-band maximum (VBM). The VBM of most III-V compounds consists mostly of anion *p* and a smaller amount of cation *p* orbitals. However, in boron compounds, the B atom participates actively in the formation of the VBM. The strong hybridization of the B and P *p*-states is clearly visible in the partial densities of states (Figure 5).



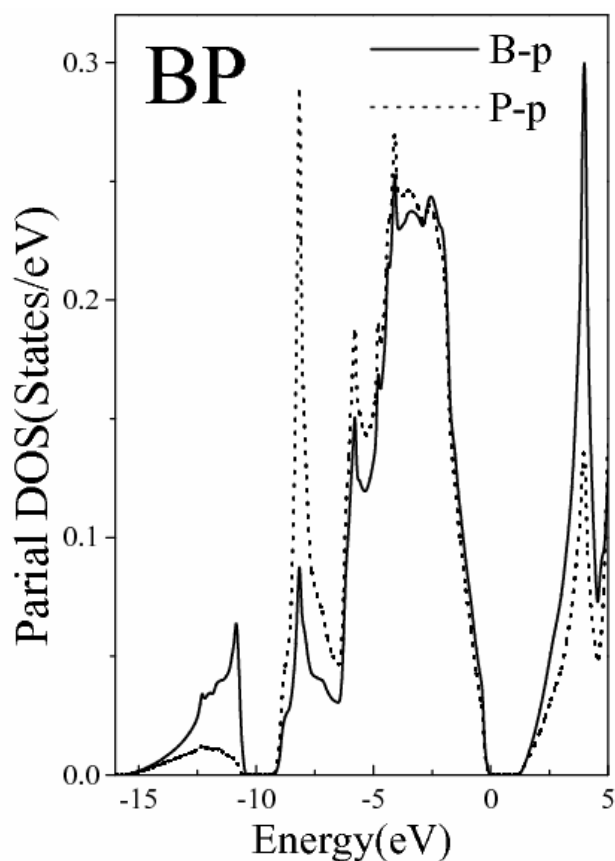
**Figure 2.** Band structure of BP.



**Figure 3.** Band structure of BBi.



**Figure 4.** Charge density plot of the  $X_{1c}$  and  $X_{3c}$  conduction bands of BP.

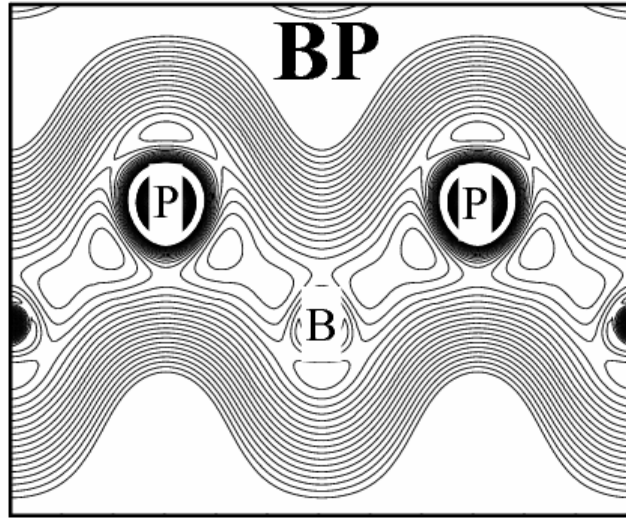


**Figure 5.** Partial density of states of  $p$ -states of BP.

## Bonding properties

Other intriguing features of boron compounds are their anomalous bond properties compared to III-V compounds. According to the Phillips scale of electronegativities B is more electronegative than P, As, Sb and Bi. Tight binding and ab initio pseudopotentials calculations have pointed out that the effective charges of BP, BAs, BSb and BBi are negative. This result is opposite to that found in common III-V semiconductors.

As shown in Figure 6, the charge density reveals two distinct local maxima (double humps) along the bond as in the case of IV compounds (i.e. C and Si). The boron compounds show strong covalency and then are reminiscent to the VI family in their bonding properties. These results hold for the other boron compounds BAs, BSb, and BBi, in which the B atom is an anion instead of a cation. This reversal of the anion and the cation roles has been discussed previously by Wentzcovitch et al [17,20] and Ferhat et al [18,19], and predicted by Phillips scale of electronegativities [34] since the first-row element B is more electronegative than P, As, Sb and Bi.



**Figure 6.** Total valence charge density plot of BP.

## Pressure effects

The effect of hydrostatic pressure on the electronic properties of boron compounds have been theoretically addressed recently by Bouhafs et al [35] and Azzi et al [15], however no experimental work has been devoted to this.

Table 3 gives the calculated pressure coefficient ( $\Gamma_{15v} \rightarrow \Gamma_{1c}$ ) and band gap volume deformation of BP, BAs and BSb, and BBi. The boron compounds have weaker (stronger) pressure coefficient (band gap volume deformation potential) compared to other III-V due to the shorter bond lengths. Other feature seen in the effect of pressure is that the direct band-gap pressure coefficient of the  $\Gamma_{1c}$  band in boron compounds is relatively constant, when the group V atoms are changed from P to Bi.

**Table 3.** Calculated band gap pressure ( $a_p$ ) and deformation ( $a_v$ ) potentials for the  $\Gamma_{15v} \rightarrow \Gamma_{1c}$  transition for zinc-blende boron compounds.

	$a_p$ , eV / Mbar	$a_v$ , eV
<b>BP</b>	9.05 <sup>a</sup> , 8.84 <sup>b</sup>	-15.44 <sup>a</sup> , -15.2 <sup>b</sup>
<b>BAs</b>	9.07 <sup>a</sup> , 8.88 <sup>b</sup>	-12.75 <sup>a</sup> , -12.88 <sup>b</sup>
<b>BSb</b>	5.76 <sup>a</sup> , 7.13 <sup>b</sup>	-6.13 <sup>a</sup> , -7.7 <sup>b</sup>
<b>BSb</b>	10 <sup>c</sup>	

<sup>a</sup> [15], <sup>b</sup> [35], <sup>c</sup> [9].

Theoretical works on the high pressure phases of BP, BAs, and BSb have been studied by Wentzcovith et al [20] and Zaoui et al [36]. These compounds were shown to favour the rocksalt (RS) phase over the  $\beta$ -Sn phase, even though BP, BAs, and BSb are the least ionic of III-V zinc-blende semiconductors. The calculated [20,36] transition pressure from ZB to RS structures are 160, 110, and 53 GPa for BP, BAs, and BSb, respectively. These are much larger than the pressures of the transition observed in most III-V compounds.

## **Alloyng III-V compounds with boron**

Recent interest has been registered for III-V boron alloys, because they offer new opportunities in band gap engineering, e.g. for solar cell and infrared applications. Investigation of dilute BGaAs and BAIsAs have been made on films grown via both molecular beam epitaxy (MBE) and metal organic chemical vapour deposition (MOCVD). It is expected that the incorporation of boron in III-V semiconductors, will induce a strong perturbation in the electronic and structural properties of these alloys, since boron has highly dissimilar properties than the remaining III and V elements of the Periodic Table.

On the other hand, only few theoretical calculations have been addressed to study the structural and electronic properties of III-V boron alloys. The most important results concerning optical properties of III-V compounds with boron are summarized as follows:

- (a) all III-V boron alloys show strong band gap bowing ( $b > 1$  eV), i.e. 4.3 for B GaN [8], and 3.5 and 2.3 eV for B GaAs [37,38], except B GaSb (0.65 eV) and B PAs (0.87 eV) [15];
- (b) the mixed cation boron compounds containing N or In elements show huge band gap bowing (6.3 – 13.4 eV) [15];
- (c) the mixed anion boron BNSb shows giant optical band gap bowing ( $b = 19.78$  eV). Similar huge band gap bowing was found previously for highly mismatched semiconductor alloys [39,40] containing nitrogen like GaAsN, InAsN, GaNP and GaSbN;
- (d) the III-V boron alloys are characterized by a strong competition between structural (volume deformation and structural relaxation) and chemical (charge transfer) effects. For common cation alloys the volume deformation dominates charge transfer effects, and structural relation is relatively weak, while for common anion alloys, the structural effect appears to control the total optical band gap bowing.

## Dynamical properties

Recent ab initio pseudopotentials works [11-13] have addressed the dynamical properties of boron compounds. The calculated macroscopic dielectric constant and Born effective charge, also referred as the dynamical effective charge (different from the static charge), are given in Table 4 for BP, BAs, BSb, and BBi. The calculated effective charge for all the boron compounds is negative, while the III-V compounds have a positive effective charge. Again this might be seen as an indication that the B atom plays the role of ‘the anion’ with respect to the effective charge of BP, BAs, BSb, and BBi.

The calculated phonon frequencies for high symmetry points in the ZB structure are given in Table 5, the calculated phonon dispersion curves for BP as prototype of boron compounds are given in Figure 7.

**Table 4.** Calculated macroscopic dielectric constant  $\epsilon_{\infty}$ , and Born effective charge  $Z$  of the zinc-blende boron compounds, experimental results (absolute value) are given in parenthesis.

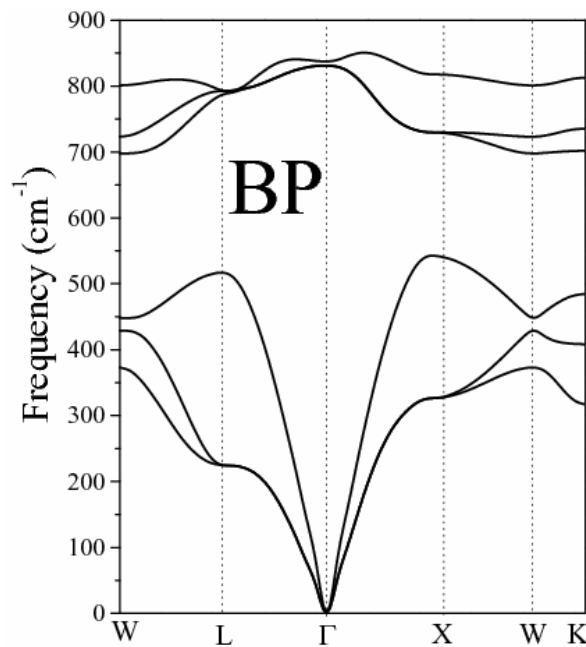
	BP	BAs	BSb	BBi
$\epsilon_{\infty}$	9.37 <sup>a</sup> (9.6 <sup>b</sup> )	9.65 <sup>a</sup>	11.3 <sup>a</sup>	14.9 <sup>c</sup>
$Z$	-0.75 <sup>a</sup> (1.34 <sup>d</sup> )	-0.57 <sup>a</sup>	-1.30 <sup>a</sup>	-1.14 <sup>c</sup>

<sup>a</sup> [11], <sup>b</sup> [41], <sup>c</sup> [13], <sup>d</sup> [42].

**Table 5.** Calculated phonon frequencies at high symmetry points for boron compounds, experimental results are given in parenthesis.

	BP	BAs	BSb	BBi
$\Gamma_{LO}$	837 <sup>a</sup> (829 <sup>b</sup> )	710 <sup>a</sup> (714 <sup>c</sup> )	621 <sup>a</sup>	560 <sup>d</sup>
$\Gamma_{TO}$	813 <sup>a</sup> (799 <sup>b</sup> )	708 <sup>a</sup>	611 <sup>a</sup>	550 <sup>d</sup>
$X_{LO}$	818 <sup>a</sup>	748 <sup>a</sup>	644 <sup>a</sup>	
$X_{LA}$	542 <sup>a</sup>	326 <sup>a</sup>	233 <sup>a</sup>	
$X_{TO}$	729 <sup>a</sup>	640 <sup>a</sup>	568 <sup>a</sup>	
$X_{TA}$	326 <sup>a</sup>	201 <sup>a</sup>	138 <sup>a</sup>	
$L_{LO}$	792 <sup>a</sup>	716 <sup>a</sup>	626 <sup>a</sup>	
$L_{LA}$	516 <sup>a</sup>	313 <sup>a</sup>	226 <sup>a</sup>	
$L_{TO}$	787 <sup>a</sup>	683 <sup>a</sup>	593 <sup>a</sup>	
$L_{TA}$	224 <sup>a</sup>	141 <sup>a</sup>	95 <sup>a</sup>	

<sup>a</sup> [11], <sup>b</sup> [42], <sup>c</sup> [28], <sup>d</sup> [13].



**Figure 7.** Phonon dispersion of BP.

The most important results concerning III-V compounds with boron are summarized as follows:

- (a) as compared to other III-V compounds where the TO and LO phonons show pronounced dispersive behaviour, in BP, BAs, BSb, and BBi, the TO and LO phonons modes are weakly dispersive;
- (b) the LO-TO splitting at the zone centre is weak, compared to other III-V compounds, which reflects the strong bonding of these compounds.

## Summary

We have surveyed in what bulk III-V boron compounds and their alloys are physically different from conventional III-V semiconductors:

- (a) the boron compounds have small lattice constants, significant bulk moduli, and elastic constants compared with the other III-V compounds;
- (b) the minimum gap of boron compounds is found close to X point ( $\Delta_{\min}$  is close to X), except BBi;
- (c) the lowest conduction band at X point is  $X_{3c}$  instead of  $X_{1c}$  as was found in most III-V semiconductors;
- (d) the lowest conduction band at  $\Gamma$  point is  $\Gamma_{15c}$  instead of  $\Gamma_{1c}$  band, in contrast to other III-V compounds where the  $\Gamma_{1c}$  state is below the  $\Gamma_{15c}$  state;

- (e) the boron compounds are characterized by a small splitting at X point ( $X_{3v}-X_{1v}$ ) compared with III-V compounds;
- (f) the boron compounds are characterized by a strong  $p$ - $p$  mixing in the valence-band maximum, in contrast with most III-V compounds;
- (g) the boron compounds show strong covalency and then are reminiscent to the VI family in their bonding properties;
- (h) the boron compounds have weaker (stronger) pressure coefficient (band gap volume deformation potential) compared to other III-V;
- (i) all III-V boron alloys show strong band gap bowing, particularly the mixed cation boron compounds containing N or In elements show huge band gap bowing;
- (j) the calculated effective charge for all the boron compounds is negative, while the III-V compounds have a positive effective charge;
- (k) in boron compounds, the TO and LO phonons modes are weakly dispersive as compared to other III-V compounds where the TO and LO phonons show pronounced dispersive behaviour.
- (l) for boron compounds, the LO-TO splitting as the zone centre is weak compared to other III-V compounds.

## References

1. Shan, W., Walukiewicz, W., Wu, J., Yu, K.M., Ager III, J.W., Li, S.X., Haller, E.E., Geisz, J.F., Friedman, D. J., and Kurtz, S.R., 2003, *J. Appl. Phys.*, **93**, 2696.
2. Leibiger, G., Gottschalch, V., Riede, V., Schubert, M., Hilfiker, J.N., and Tiwald, T.E. 2003, *Phys. Rev. B*, **67**, 195205.
3. Gottschalch, V., Leibiger, G., and Benndorf, G. 2003, *J. Cryst. Growth*, **248**, 468.
4. Saidi, F., Hassen, F., Mareef, H., Dumont, H., and Monteil, Y. 2006, *Mat. Sci. & Eng. C*, **26**, 236.
5. Dalui, S., Das, S.N., Hussain, S., Paramanik, D., Verma, S., and Pal, A.K. 2007, *J. Cryst. Growth*, **305**, 149.
6. Meradji, H., Drablia, S., Ghemid, S., Belkhir, H., Bouhafs, B., and Tadjer, A. 2004, *Phys. Status Solidi B*, **241**, 2881.
7. Zaoui, A., Kacimi, S., Yakoubi, A., Abbar, B., and Bouhafs, B. 2005, *Physica B*, **367**, 195204.
8. Escalanti, L., and Hart, G.L.W. 2004, *Appl. Phys. Lett.*, **84**, 705.
9. Madouri, D., and Ferhat, M. 2005, *Phys. Status Solidi B*, **242**, 2856.
10. Chimot, N., Even, J., Folliot, H. and Loualiche, S. 2005, *Physica B*, **364**, 263.
11. Touat, D., Ferhat, M., and Zaoui, A. 2006, *J. Phys.: Condens. Matter*, **18**, 3647.
12. Deligoz, E., Colakoglu K., Ciftci, Y.O., and Ozisik, H. 2007, *Com. Mat. Sci.*, **39**, 533.
13. Bouamama, K., Djemia, P., Lebga, N., and Kassali, K. 2007, *High Press. Res.*, **27**, 269.
14. Jenichen, A., and Engler, C., 2007, *Phys. Status Solidi B*, **244**, 1957.
15. Azzi, S., Zaoui, A., Ferhat, M. 2007, *Solid State Commun.*, **144**, 245.
16. Garcia, A., and Cohen, M.L. 1993, *Phys. Rev. B*, **47**, 4215.

17. Wentzcovitch, R.M., Chang, K.J., and Cohen, M.L. 1986, *Phys. Rev. B*, **34**, 1071.
18. Ferhat, M., Zaoui, A., Certier, M., and Aourag, H. 1998, *Physica B*, **252**, 229.
19. Bouhafs, B., Aourag, H., Ferhat, M., and Certier, M. 1999, *J Phys.: Condens. Matter*, **11**, 5781.
20. Wentzcovitch, R.M., Cohen, M.L., and Lam, P.K. 1987, *Phys. Rev. B*, **36**, 6058.
21. Wang, S.Q., and Ye, H.Q. 2003, *Phys. Status Solidi B*, **240**, 45.
22. Golikova, O.A. 1979, *Phys. Status Solidi A*, **51**, 11.
23. Surh, M.P., Louie, S.G., and Cohen, M.L. 1991, *Phys. Rev. B*, **43**, 9126.
24. Ferhat, M., and Zaoui, A. 2006, *Phys. Rev. B*, **73**, 115107.
25. Ferhat, M., and Zaoui, A. 2006, *Appl. Phys. Lett.*, **88**, 161902.
26. Numerical Data and Functional Relationships in Science and Technology. Crystal and Solid States physics, Volume III of Landolt–Börnstein, O. Madelung (Ed.). 1972, Springer, Berlin.
27. Wettling, W., and Windscheif, J. 1984, *Solid State Commun.*, **50**, 33.
28. Greene, R.G., Luo, H., Ruoff, A.L., Trail, S.S., and Di Salvo Jr, F. 1994, *Phys Rev. Lett.*, **73**, 2476.
29. Ferhat, M., Bouhafs, B., Zaoui, A., and Aourag, H. 1998, *J. Phys.: Condens. Matter*, **10**, 7995.
30. Wang, S.Q., and Ye, H.Q. 2002, *Phys. Rev. B*, **66**, 235111.
31. Archer, R.J., Koyama, R.Y., Loebner, E.E., and Lucas, R.C. 1964, *Phys. Rev. Lett.*, **12**, 538.
32. Wang, C.C., Cardona, M., and Fischer, A.G. 1964, *RCA Rev.*, **25**, 159.
33. Chu, T.L., and Hyslop, A.E. 1974, *J. Electrochem. Soc.*, **121**, 412.
34. Phillips, C. 1973, *Bonds and Bands in Semiconductors*, Academic Press, New York.
35. Bouhafs, B., Aourag, H., and Certier, M. 2000, *J. Phys.: Condens. Matter*, **12**, 5655.
36. Zaoui, A., and Ferhat, M. 2001, *Phys. Status Solidi B*, **225**, 15.
37. Zaoui, A., and Haj Hassan, F.E. 2000, *J. Phys.: Condens. Matter*, **13**, 253.
38. Hart, G.L.W., Zunger, A. 2000, *Phys. Rev. B*, **62**, 13522.
39. Geisz, J.F., Friedman, D.J., Olson, J.M., Kurtz, S.R., Reedy, R.C., Swartzlander, A.B., Keyes, B.M., and Norman, A.G. 2000, *Appl. Phys. Lett.*, **76**, 1443.
40. Vurgaftman, I., and Meyer, J.R., 2003, *J. Appl. Phys.*, **94**, 3675.
41. Belabbes, A., Ferhat, M., and Zaoui, A. 2006, *Appl. Phys. Lett.*, **88**, 152109.
42. Landolt-Börnstein New York Series, Group III, Volume 17a, O. Madelung (Ed.). 1982, Springer, Berlin.
43. Sanjurjo, J.A, Lopez-Cruz, E., Vogl, P., and Cardona, M. 1983, *Phys. Rev. B*, **28**, 4579.