

Band Structure, Metallization and Superconducting Transition of Group III-V Semiconductors *AIP* and *AlAs* under High Pressure

V. Benaline Sheeba¹, C. Nirmala Louis^{2,*}

¹Udaya School of Engineering, Vellamodi, Kanyakumari District, Tamil Nadu, India

²Research Center in Physics, Holy Cross College, Nagercoil, Tamil Nadu, India

*Corresponding Author: nirmala_louis@yahoo.co.in

Copyright © 2013 Horizon Research Publishing All rights reserved.

Abstract The results of a full potential linear muffin-tin orbital (FP-LMTO) study on the electronic properties of cubic zinc blende type group III-V semiconductors *AIP* and *AlAs* under pressure are presented. The equilibrium lattice constant, bulk modulus, pressure derivative of bulk modulus and the phase transition pressure at which the compounds undergo structural phase transition from ZnS to NaCl and NaCl to CsCl are predicted from the total energy calculations. The ground state properties and band gap values are compared with the experimental results. At normal pressure *AIP* and *AlAs* are indirect bandgap semiconductors. When the pressure is increased there is enhanced overlapping between the wave functions of the neighbouring atoms. As a result the widths of the valence and empty conduction bands increase. These changes lead to the narrowing and indirect closing of band gaps in *AIP* and *AlAs* (metallization). On further increase of pressure, *AIP* and *AlAs* become superconductors, and these materials come under the class of electron-phonon-mediated high pressure superconductors. The superconducting transition temperatures (T_c) of *AIP* and *AlAs* are obtained as a function of pressure for CsCl structure. It is also confirmed that the metallization, structural phase transition and onset of superconductivity do not occur simultaneously in these compounds.

Keywords Band Structure, Density of States, Phase Transition, Metallization, Superconductivity, *AIP* and *AlAs*, High Pressure

1. Introduction

The enormous properties like ductility, light weight and high strength of aluminum compounds makes it the best choice for many areas of constructive as well as other important engineering applications^[1]. The study of materials at high pressure is gaining importance because of recent refinements of the diamond anvil technique^[2] and the

observation that materials often exhibit new crystal phases and novel behaviour under high pressure. Group III-V semiconductors *AIP* and *AlAs* have been extensively studied because they are considered important technological materials in electronic and opto electronic applications^[3-6]. The effect of pressure on the electronic properties of group III-V compounds can be investigated experimentally in many ways^[7,8]. The technological applications of all the above compounds require significant progress in the fundamental understanding of their behaviour at normal and high pressures. Generally aluminum compounds (*AIP* and *AlAs*) crystallize in zinc blende (ZnS) structure. ^[9,10]

In our calculation we have chosen zinc blende structure as the normal pressure structure of *AIP* and *AlAs* compounds. *AIP* and *AlAs* are characterized by indirect band gap. ^[9] *AIP* and *AlAs* are used as an active material in the manufacture of opto electronic devices and also in LEDs etc. They act as a promising candidate in semiconductor technology due to its wide and indirect bandgap ^[11]. Also it has gained importance in the technology for opto electronic applications in the short wave length range as well as for high temperature, high power and high frequency electronic devices. In particular *AlAs* is a basic material for light emitting diodes, lasers in the blue and ultraviolet range of the spectrum, optical pumping structures, photo detectors and hetero structure^[1,2]. Subjecting *AIP* and *AlAs* to high pressure leads to pressure induced metallization, structural phase transition and superconducting transition.

The band gap value for *AIP* and *AlAs* were experimentally measured by Hellwege *et al*^[12]. Theoretically numerous results on the band structure of *AIP* and *AlAs* exist^[9-11]. Wang *et al*^[9] presented the mechanical and electrical properties of twelve III-V semiconductors under pressure using Plane wave Pseudopotential method. There is no high pressure studies related to metallization and superconductivity in both *AIP* and *AlAs*. This motivated us to take up the present investigation of these compounds under high pressure. In this work self consistent full potential linear muffin tin orbital method (FP-LMTO) is employed to study

the effect of pressure on the band structure of these compounds.[13] We have analyzed the phenomena of metallization and superconductivity for high pressure (*CsCl*) structure of these materials. It is hoped that this analysis will enable us to make some general statement regarding the path to high T_c superconductivity in covalent compounds. In Section 2, we give the details of the calculational procedure, electronic band structure and density of states corresponding to various pressures. The ground-state properties, structural phase transition, metallization and superconducting transition temperature T_c and its variation under pressure are discussed in Section 3. Concluding remarks are given in Section 4.

2. Band Structure and Density of States

2.1. Calculational Procedure

The electronic band structure calculations were performed for *AIP* and *AlAs* corresponding to different reduced volumes in *ZnS*, *NaCl* and *CsCl* structures, by the first-principle FP-LMTO method with in generalized gradient approximation (GGA) [14]. We have used the exchange-correlation potential of Ceperley and Alder as parametrized by Perdew and Zunger [15]. similar to our earlier studies on *ZnSe* and *CdSe* the details of the FP-LMTO method are well described in the literature[13] and we give here only the calculational details. The electronic configurations of *Al* and *P* are $[\text{Ne}] 3s^2 3p^1 3d^{10}$ ($Z = 13$) and $[\text{Ne}] 3s^2 3p^3$ ($Z = 15$) respectively, and for *As* it is $[\text{Ar}] 4s^2 4p^3$ ($Z = 33$). The valence electronic configurations chosen in our calculations are $3s^2 3p^1$ for *Al*, $3s^2 3p^3$ for *P* and $4s^2 4p^3$ for *As*. There are 8 valence electrons contributing to the valence bands[13]. The final energy convergence is within 10^{-5} Ry. The calculated total energies were fitted to Murnaghan's equation of state (EOS) [16], to determine the phase-transition pressure and other ground-state properties.

2.2. Band Structure of AIP and AlAs under Pressure

The band structures of *AIP* and *AlAs* were computed for various reduced volumes ranging from $V/V_0=1.0$ to 0.3 in steps of 0.05. Even though we have obtained the band structure for V/V_0 values from 1.0 to 0.3, we have presented here the band structures of *AIP* and *AlAs* along the symmetry directions Γ - X - W - L - Γ - K and the corresponding density of states of *AIP* and *AlAs* (Figs.1 to 8).The volume compressions corresponding to $V/V_0=1.0$ and $V/V_0=0.52$ for *AIP*, and $V/V_0=1.0$ and $V/V_0=0.5$ for *AlAs* only. The overall topology of the band structure of *AIP* and *AlAs* at $V/V_0=1.0$ (Figs.1 and 3) is same as that of previous calculations^[9]. A single band nearer to origin arises from $3s^2$ electrons of P (Fig.1) and $4s^2$ electrons of As (Fig.3). The three bands appearing below the Fermi level are due to the $3s^2$, $3p^1$ electrons of *Al* and $3p^3$ electrons of *P* (Fig.1). Similarly in

Fig.3, the three bands positioned below the Fermi level are due to $3s^2$, $3p^1$ electrons of *Al* and $4p^3$ electrons of *As*. The empty conduction bands above the Fermi level are due to $3p$, $3d$ states of *Al* and $3d$, $3p$ states of *P* (Fig.1) and $4d$, $4p$ states of *As* (Fig.3).

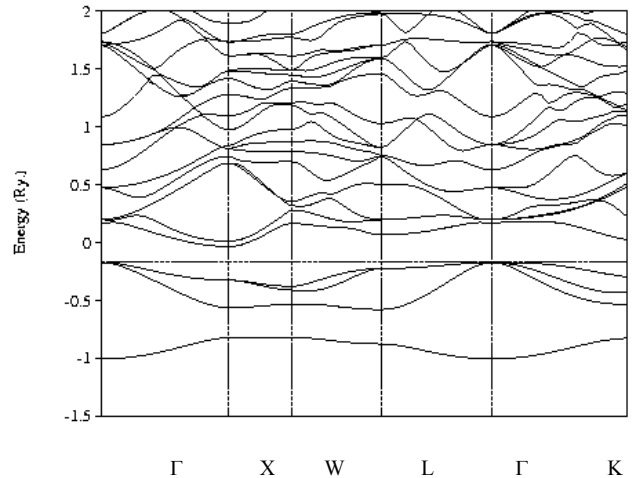


Figure 1. Band structure of *AIP* at $V/V_0=1$ in zinc blende structure (normal pressure)

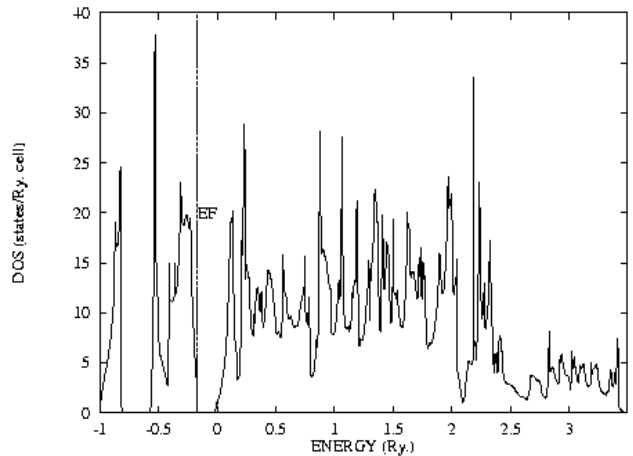


Figure 2. Density of states of *AIP* at $V/V_0=1$ in zinc blende structure (normal pressure)

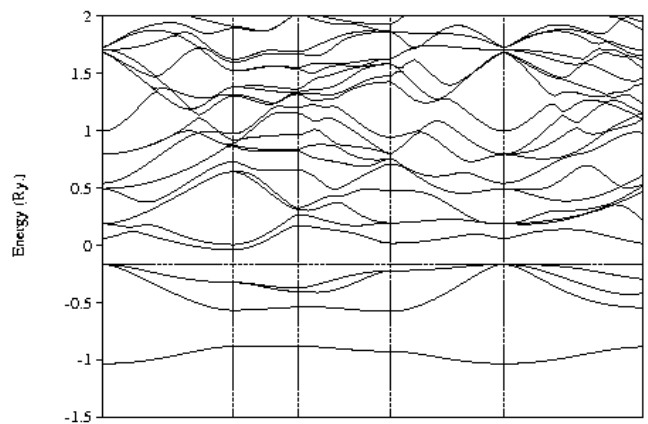


Figure 3. Band structure of *AlAs* at $V/V_0=1$ in zinc blende structure (normal pressure)

At normal pressure, the band gap of *AIP* is indirect with valence band maximum at Γ point and conduction band minimum at X point with band gap value 2.1 eV. In the case of *AlAs*, band gap is indirect with a value of 2.2 eV with valence band maximum at Γ point and conduction band minimum at X point. The calculated energy gaps are in

agreement with the experimental values[12] for both *AIP* and *AlAs* (Table 1). As pressure increases the width of the valence band and the empty conduction band get widened. These changes leads to the narrowing of the band gap under pressure (Figs. 5 and 7).

Table 1. Equilibrium lattice constant (a_0), bulk modulus (B_0) and its pressure derivative (B_0') of *AIP* and *AlAs* in *ZnS* structure

Ground State Properties	AIP			AlAs		
	Present work	Experimental works [4,12]	Previous theoretical works[9,10]	Present work	Experimental works[4,12]	Previous theoretical works[9,10]
ao a.u.	10.327	10.432	10.034	10.7	10.825	10.547
Bo bar	0.86	0.89	0.74	0.82	0.84	0.76
Bo1	4.037	4.143	3.954	4.182	4.423	4.142
Eg eV	2.1	2.4	1.92	1.95	2.2	1.84

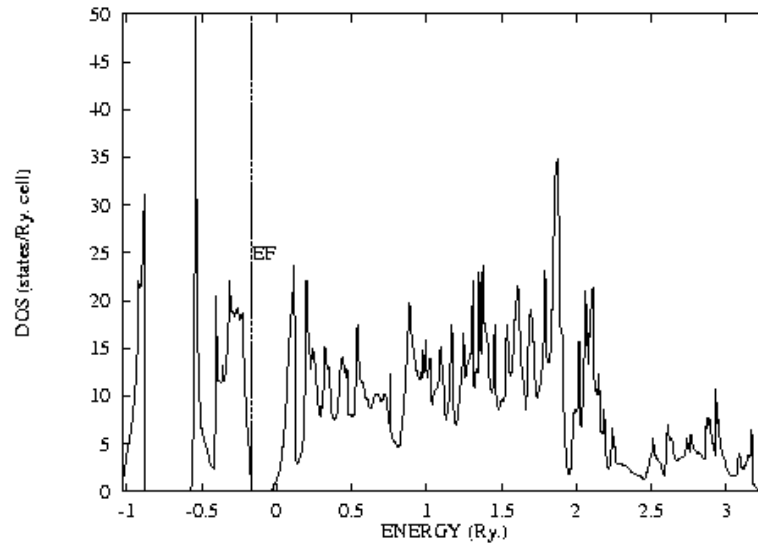


Figure 4. Density of states of *AlAs* at $V/V_0=1$ in zinc blende structure (normal pressure)

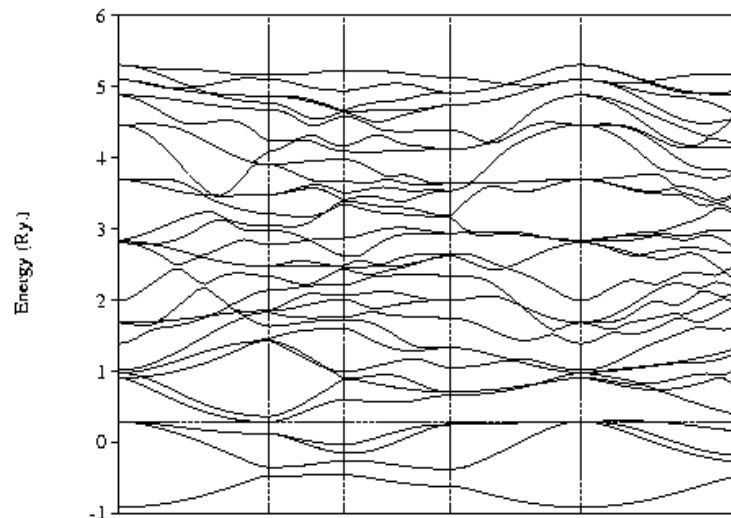


Figure 5. Band structure of *AIP* at $V/V_0=0.52$ in *CsCl* structure (pressure = 2.275 Mbar)

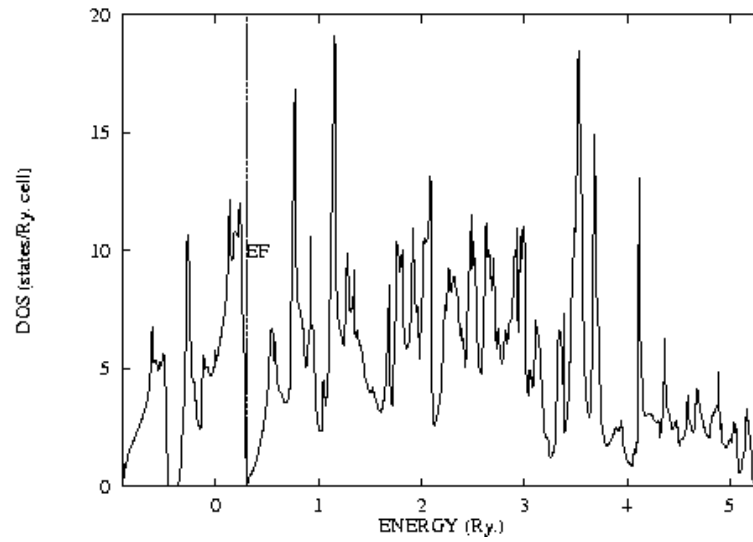


Figure 6. Density of states of *AIP* at $V/V_0=0.52$ in *CsCl* structure (Pressure = 2.275 Mbar)

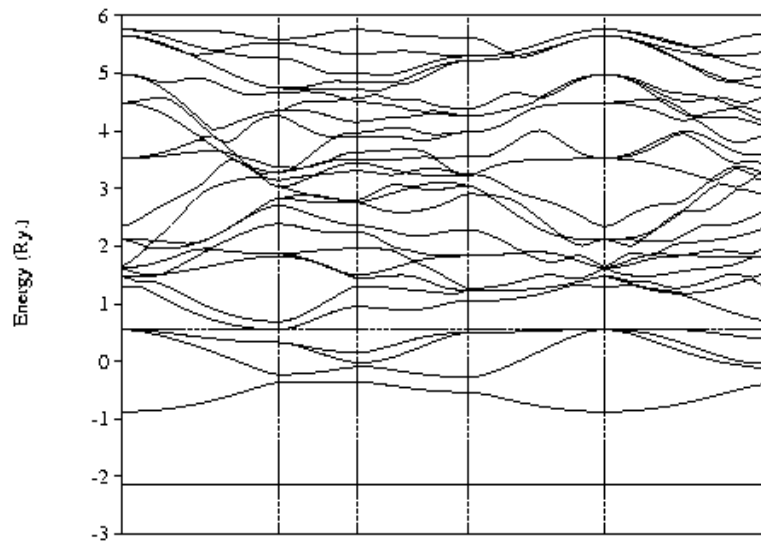


Figure 7. Band structure of *AIPs* at $V/V_0=0.5$ in *CsCl* structure (pressure = 2.44 Mbar)

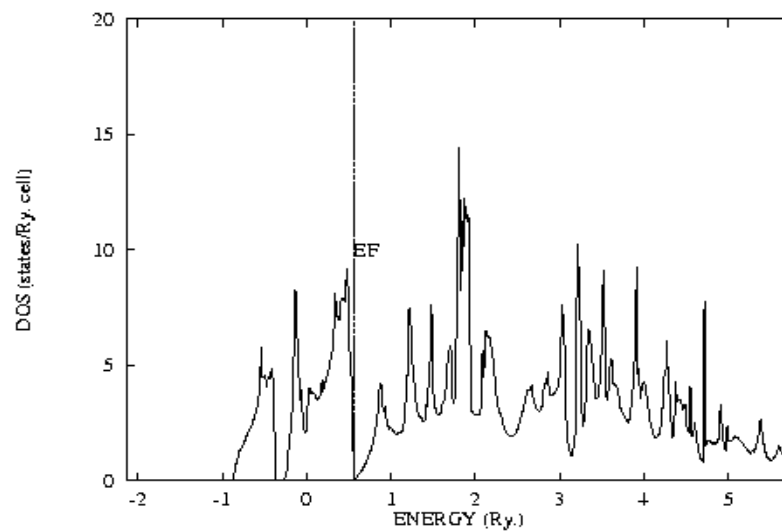


Figure 8. Density of states *AIPs* at $V/V_0=0.5$ in *CsCl* structure (pressure = 2.44 Mbar)

2.3. Density of States under Pressure

The density of states (DOS) (states/Ry.) calculations for all the reduced volumes have been carried out. The density of states (DOS) histogram of *AlP* corresponding to normal pressure is shown in Fig.2. At normal pressure the levels arising from $3s^2$ electrons of *Al* give the long spike near the origin. The short spikes near the Fermi energy are due to $3s^2$, $3p^3$ electrons of *P* and $3p^1$ electron of *Al*. The short peaks above the Fermi energy E_F are due to the $3p$, $3d$ states of *Al* and $3d$, $3p$ states of *P*. The density of states (DOS) histogram of *AlAs* corresponding to normal pressure is shown in Fig.4. At normal pressure the levels arising from $3s^2$ electrons of *Al* give the long spike near the origin. The short spikes near the Fermi energy are due to $4s^2$, $4p^3$ electrons of *As* and $3p^1$ electron of *Al*. The short peaks above the Fermi energy E_F are due to the $3p$, $3d$ states of *Al* and $4d$, $4p$ states of *As*. The general features of the band structure and density of states (Figs 1-8) are similar to that of the alkali halides [17].

This trend is changed under high pressure. The increase of pressure leads to the broadening of bands which results in the decrease of density of states value in most of the energy regions and also increase in the width of the valence band and empty conduction bands. When pressure increases the value of E_F increases whereas no density of states is available at the Fermi level up to metallization pressure. In Fig.6, there is appreciable value for $N(E_F)$ at $V/V_o = 0.52$, for *AlP* in *CsCl* structure, which indicates metallization in *AlP*. In Fig.8, there is appreciable value for $N(E_F)$ at $V/V_o = 0.5$, for *AlAs* in *CsCl* structure, which indicates metallization in *AlAs*. Further increase in pressure leads to enhanced density of states at the Fermi level which induces superconductivity [13].

3. Results and Discussion

3.1. Ground State Properties

The ground state properties and structural phase transitions of *AlP* and *AlAs* are studied from their total energies obtained from our calculation. The total energy is calculated as a function of reduced volume (V/V_o) for *ZnS*, *NaCl* and *CsCl* phases of *AlP* and *AlAs*. Here, V_o is the experimental equilibrium volume corresponding to the experimental equilibrium lattice constant. The calculated total energies were fitted to Murnaghan's equation of state [16]

$$P = 1.5B_o [(V_o/V)^{7/3} - (V_o/V)^{5/3}] [1 + 0.75 (B_o^{-1} - 4) \{(V_o/V)^{2/3} - 1\}] \quad (1)$$

to obtain the equilibrium lattice constant and other ground state properties. The relation between reduced volume and lattice constant is shown in Fig.9. Here lattice constant decreases with decrease of reduced volume. The relation between reduced volume and pressure is shown in Fig.10. When reduced volume decreases pressure increases. The variation in the total energy as a function of reduced volume for *AlP* is shown in Fig. 11. From this figure, it is found that, in *AlP*, up to $V/V_o = 0.73$, *ZnS* structure has the lowest energy and on further reduction of volume *NaCl* structure becomes more stable in energy than the *ZnS* structure. Also up to $V/V_o = 0.62$, *NaCl* structure has the lowest energy and on further reduction of volume *CsCl* structure becomes more stable in energy than the *NaCl* structure.

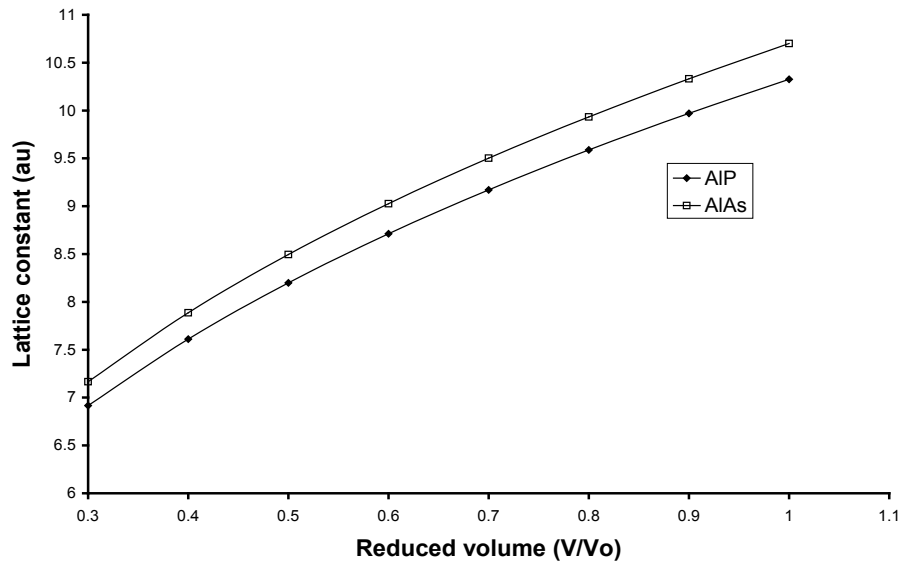


Figure 9. Relation connecting reduced volume and lattice constant

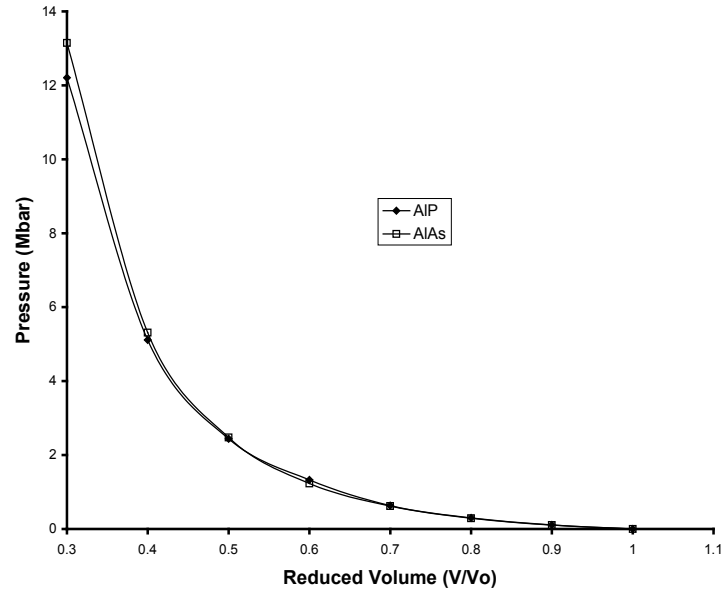


Figure 10. Relation connecting reduced volume and pressure

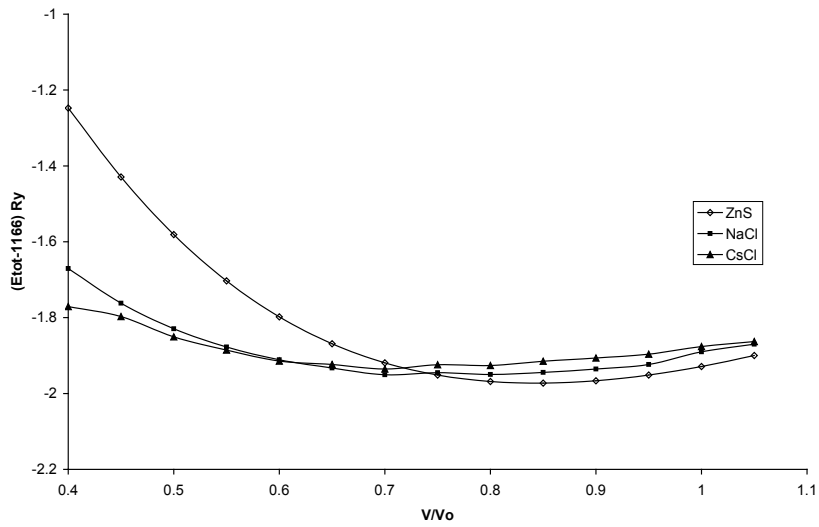


Figure 11. Relation connecting total energy and reduced volume curve of AIP

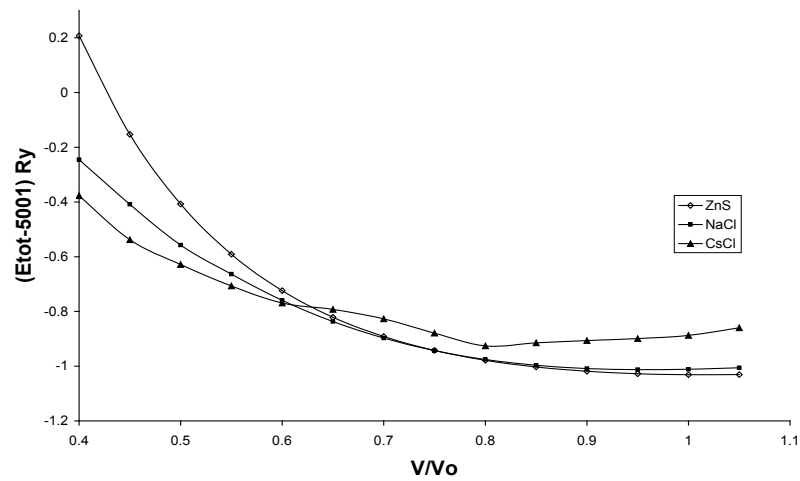


Figure 12. Relation connecting total energy and reduced volume curve of AlAs

The variation in the total energy as a function of reduced volume for *AlAs* is shown in Fig. 12. From this figure, it is found that, in *AlAs*, up to $V/V_0 = 0.76$, *ZnS* structure has the lowest energy and on further reduction of volume *NaCl* structure becomes more stable in energy than the *ZnS* structure. Also up to $V/V_0 = 0.625$, *NaCl* structure has the lowest energy and on further reduction of volume *CsCl* structure becomes more stable in energy than the *NaCl* structure. In Table 1, the equilibrium lattice constant (a_0), band gap (E_g), bulk modulus (B_0) and its pressure derivative (B_0^1) values are compared with experimental and previous theoretical works[1-10]. From Table 1, it is observed that one gets larger lattice constant corresponding to smaller bulk modulus. Our estimated bulk modulus of *AlAs* is less than that of *AIP*, as a result compressibility is higher for *AlAs* than *AIP* (Fig.10). Thus, it is noted that the compressibility decreases as the size of the anion decreases. This is the general trend in alkali halides^[17], which is confirmed now for *AIP* and *AlAs*.

3.2. Structural Phase Transition

In our calculation we have chosen the *ZnS* structure for both *AIP* and *AlAs* at ambient pressure. The phase stability of the B3 (*ZnS*), B1 (*NaCl*) and B2 (*CsCl*) structures of *AIP* and *AlAs* is analysed using the enthalpy calculation [13]. The enthalpy $H(P)$ is defined by

$$H(P) = E_{\text{tot}}(P) + PV(P) \quad (2)$$

and the transition pressure corresponding to the phase transition from B3 to B1 is obtained from the relation

$$H_{B3}(P) = H_{B1}(P) \quad (3)$$

where H_{B3} and H_{B1} are the enthalpies of the B3(*ZnS*) and B1(*NaCl*) phases respectively. Similarly $H_{B1}(P) = H_{B2}(P)$ where H_{B1} and H_{B2} are the enthalpies of the B1(*NaCl*) and B2(*CsCl*) phases respectively. The phase transition pressure (P_T) and the corresponding reduced volume $(V/V_0)_T$ estimated in our calculation are given in Table.2.

For *AIP* and *AlAs*, our calculated phase transition pressure is in good agreement with the experimental and previous theoretical results. The mechanism for the phase transition is

a geometric effect involving a change in the coordination number from 4 in the *ZnS* phase to 6 in the *NaCl* phase and to 8 in the *CsCl* phase under pressure[17].

3.3. Metallization

At normal pressure *AIP* and *AlAs* are wide gap semiconductors. With the increase of the pressure, the band gap decreases and at a particular pressure, there is a closing of the band gap. The band structure and density of states corresponding to metallization of *AIP* and *AlAs* are shown in Figs. 5to 8 respectively. In *AIP* and *AlAs*, the metallization occurs through indirect closing of the band gap between valence band maximum at Γ point and conduction band minimum at X point. The metallization volume of *AIP* is $V/V_0=0.52$ (*CsCl* structure), which corresponds to the pressure $P_M = 2.275$ Mbar. In the case of *AlAs* the indirect closure of the band gap between Γ and X point takes place at the reduced volume $V/V_0=0.50$ (*CsCl* structure), the corresponding metallization pressure is 2.44 Mbar.

The metallization pressure calculated for *AlAs* is greater than that of *AIP* (Table 2). This means, in group III-V compounds, metallization pressure increases with the increasing size of the group - V element. This trend is opposite to the trend observed in alkali halides having *NaCl* structure at ambient conditions (metallization pressure increases with decreasing size of alkali metal[17]). The reason for this difference is that, prior to metallization, alkali halides undergo structural transition from *NaCl* to *CsCl* structure whereas group III-V compounds undergo structural transition from *ZnS* to *NaCl* to *CsCl* structure. At the metallization pressures, the values for density of states at Fermi energy $N(E_F)$ are very small (pseudo gap), which indicate that metallization has just set in *AlAs* and *AIP* (Figs.6 and 8). Thereafter $N(E_F)$ increases slowly with pressure and becomes fairly large at a particular value of V/V_0 . The values of E_F and $N(E_F)$ corresponding to different V/V_0 are used in studying the pressure variation of superconducting transition temperature[13]. However, there are no experimental or theoretical study available for comparison at these pressures.

Table 2. Metallization, phase transition and superconducting transition pressures in *AIP* and *AlAs*

Aluminum Compound	Metallization		Phase transition ZnS to NaCl and NaCl to CsCl		Onset of superconducting transition	
	P M Mbar	(V/V ₀) M	P T Mbar	(V/V ₀) T	P S Mbar	(V/V ₀) S
AIP	2.275	0.52	0.5116	0.730	3.0	0.532
			1.084	0.620		
AlAs	2.44	0.50	0.40	0.760	3.0	0.514

3.4. Superconductivity in AIs and AIP under Pressure

The promotion of *s* electron to *d* shell in solids is one of the factors which will induce superconductivity. Under very high pressure, aluminum compounds are not only metals but also superconductors. The theory of Gaspari and Gyorfyy [18] in conjunction with McMillan's formula is used to calculate T_c .

The electron-phonon mass enhancement factor, λ is [19]

$$\lambda = \frac{N(E_F)\langle I^2 \rangle}{M\langle \omega^2 \rangle} \quad (4)$$

where M is the atomic mass, $\langle \omega^2 \rangle$ is an average of the phonon frequency square and $\langle I^2 \rangle$ is an average (over the Fermi energy) of the electron-phonon matrix element square [19].

$\langle I^2 \rangle$ (in Rydbergs) can be written as

$$\langle I^2 \rangle = 2 \sum_l \frac{(l+1)}{(2l+1)(2l+3)} M_{l,l+1}^2 \frac{N_l(E_F)N_{l+1}(E_F)}{N(E_F)N(E_F)} \quad (5)$$

where $M_{l,l+1} = -\phi_l \phi_{l+1} [(D_l(E_F)-1)(D_{l+1}(E_F)+1+2) + (E_F-V(S))S^2]$ and in this,

ϕ_l is the radial wave function at the muffin-tin sphere radius corresponding to the Fermi energy.

D_l is the logarithmic derivative of the radial wave function at the sphere boundary.

$V(S)$ is the muffin-tin potential at the sphere boundary.

S is the radius of the muffin-tin sphere.

The above quantities are taken from the band structure results.

The average of the phonon frequency square is

$$\langle \omega^2 \rangle = \frac{1}{2} \theta_D^2 \quad (6)$$

The variation of Debye temperature with pressure $\theta_D(P)$ is given by [13]

$$\theta_D(P) = \frac{\sqrt{E_F} a_o}{\sqrt{E_F^o} a} \theta_D^o \quad (7)$$

where θ_D^o , a_o and E_F^o are normal pressure quantities.

The McMillan's formula [20] used for T_c calculation,

$$T_c = \frac{\theta_D}{1.45} \exp \left[\frac{-1.04(1+\lambda)}{\lambda - \mu^* (1+0.62\lambda)} \right] \quad (8)$$

gives the good estimate of the T_c value. Here μ^* is the electron-electron interaction parameter which is estimated using the relation [21],

$$\mu^* = \frac{0.26N(E_F)}{1+N(E_F)} \quad (9)$$

where $N(E_F)$ is the density of levels per atom per eV at E_F .

With the results obtained from the self-consistent calculation, we have computed θ_D , λ , μ^* and T_c as a function of pressure using Eqs.(4 - 9). The calculated values at high pressure (*CsCl*) structure is given in Tables. 3 and 4 for *AIP* and *AlAs* respectively. As pressure increases our computed value of T_c increases and reaches a maximum value. In our calculation the highest T_c obtained in *AIP* is 5.911 K at 4.5 Mbar (Table. 3), whereas in *AlAs* the highest T_c obtained is 14.54 K at 4.5Mbar (Table. 4). The calculated T_c values depend more sensitively on changes in λ than μ^* , indicating that these compounds are electron-phonon-mediated superconductors. Similar to alkali halides and group II-VI compounds, group III-V compounds come under the class of pressure induced superconductors [13,17]. When pressure is increased T_c increases and reaches the maximum value in both the *AIP* and *AlAs*. This reflects the fact that the structural and band gap configurations play an important role in the superconducting (high T_c -max) behaviour of these compounds under high pressure. [13]

Table 3. Variation of T_c as a function of pressure for *AIP* in *CsCl* structure

Pressure P Mbar	λ	θ_D K	μ^*	T_c K
3	0.286	528	0.101	0.122
3.5	0.343	671	0.112	0.546
4	0.431	732	0.124	2.203
4.5	0.527	868	0.138	5.911

Table 4. Variation of T_c as a function of pressure for *AlAs* in *CsCl* structure

Pressure P Mbar	λ	θ_D K	μ^*	T_c K
3	0.327	573	0.113	0.289
3.5	0.418	698	0.124	1.725
4	0.522	786	0.132	5.683
4.5	0.653	912	0.140	14.54

4. Conclusion

In the present investigation, the pressure dependent band structures and density of states of *AIP* and *AlAs* are computed and the results are used to study the metallization and superconductivity under high pressure for the first time. When the pressure is increased there is enhanced overlapping between the wave functions of the neighbouring atoms. As a result the widths of the valence and empty conduction bands increase. These changes lead to the narrowing and closing of band gaps in *AIP* and *AlAs* (metallization). On further increase of pressure, *AIP* and *AlAs* become superconductors, and these materials come under the class of electron-phonon-mediated high pressure superconductors. It is also confirmed that the metallization, structural phase transition and onset of superconductivity do not occur simultaneously in aluminum compounds.

Acknowledgments

The financial support from the UGC Minor Research Project – No: MRP-4057/11 (UGC – SERO) dated August 2012 is greatly acknowledged with thanks.

REFERENCES

- [1] Jin Cai and Nanxian Chen, *Phys. Rev. B* 75, 174116 (2007).
- [2] H. Hirano, et al *J. of Phys. and Chem. of Sol.* 62,941 (2001).
- [3] L.H. Yua, K.L. Yaoa, Z.L. Liu, *Solid State Commun.*135 , 124 (2005).
- [4] Sadao Adachi, *Properties of Group.IV, III–V and II–VI Semiconductors*, John Wiley & Sons, England, 2005
- [5] I. Vurgaftman, J.R. Meyer, L.R. Ram.Mohan, *J. Appl. Phys.*, 89, 5815 (2001).
- [6] A. Bouhemadou, R. Khenata, *J. of Phys. and Chem. of Sol.*, 68, 549 (2007).
A. Lindbaum, S. Heathman, K. Litfin and Y. Meresse, *Phys. Rev.B* 63, 214101 (2001).
- [7] Samuel T. Weir, J. Akella, C. Aracne-Ruddle, Y.K. Vohra and S.A. Catledge, *Appl. Phys. Lett.* 77, 3400 (2000).
- [8] S.Q.Wang and H.Q. Ye, *Phys. Rev. B* 66, 235111 (2002).
- [9] J.Wu, W. Walukiewicz, W. Shan, K.M. Yu, J.W. Ager III, E.E. Haller, H.Lu and W.L. Schaff, *Phys.Rev. B* 66, 201403 (2002).
- [10] A.Mahmood, L.Enrique Sansores and S.Muhl, *Superficies y Vacio* 9, 259 (1999).
- [11] K.H.Hellwege and O.Madelung, *Landolt-Bornstein New series, Group III.Vol 17a*,(Berlin :Springer)1982.
- [12] C.Nirmala Louis and A.AmalRaj, *Chemical and Materials Engineering* 1(2): 43-52, 2013.
- [13] O. K. Andersen, O. Jepsen and M.Sob, in *Electronic bandstructure and its applications*, edited by M. Yussouff(Springer, Heidelberg,1987) P.1; S.Limpijumngong and W.L.Lambrecht, *Phys.Rev. B*, 63, 104103 (2001); Savrasov.S.Yu and Savrasov.D.Yu, *Phys. Rev.B*,46,12181 (1992).
- [14] D.M. Ceperley and B.J. Alder, *Phys.Rev .Lett.*45 , 566 (1980);
- [15] J.Perdew and Z. Zunger, *Phys.Rev .B*23, 5048 (1981).
- [16] F. D. Murnaghan, *Proc. Natl. Acad. Sci. USA* 30, 244 (1944).
- [17] C. Nirmala Louis and K. Iyakutti, *Phys. Stat. Sol(b)* 236, 614 (2003); *Phys. Stat. Sol(b)* 233, 339 (2002).
- [18] G.D. Gaspari and B.L. Gyorffy, *Phys .Re v. Lett* 29, 801(1972).
- [19] P. Bruesch, *Phonons- Theory and Experiments-I*, (Springer-Verlag,Berlin, 1982) p.81.
- [20] W.L. Mcmillan, *Phys. Rev.* 167, 331 (1968).
- [21] K. H. Bennemann and J.W. Garland, *AIP Conf. Proc.* 4, 103 (1972).