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BAND STRUCTURE, DENSITY OF STATES AND METALLIZATION IN GALLIUM ANTIMONIDE (*GaSb*) UNDER HIGH PRESSURE

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Abstract

The uniqueness of gallium antimonide (GaSb) and its special role in human society is closely related to its structural stability at extreme pressures. In this paper, 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 semiconductor gallium antimonide (GaSb) under pressure are presented. The equilibrium lattice constant, bulk modulus, pressure derivative of bulk modulus are predicted from the total energy calculations. The ground state properties and band gap values are compared with the experimental results. At normal pressure GaSb is indirect bandgap semiconductor with bandgap value 0.726 eV. 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 GaSb (metallization).

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Keywords: *Band structure, Density of states, gallium antimonide, Metallization.*

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1. Introduction

The enormous properties like ductility, light weight and high strength of gallium 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 and the observation that materials often exhibit new crystal phases and novel behaviour under high pressure [2]. Group III-V semiconductor *GaSb* is extensively studied because it is considered important technological material in electronic and opto electronic applications. The effect of pressure on the electronic properties of group III-V compounds can be investigated experimentally in many ways [3]. The technological applications of all the above compounds require significant progress in the fundamental understanding of their behaviour at normal and high pressures. Generally gallium compounds (*GaP, GaSb* and *GaAs*) crystallize in zinc blende (*ZnS*) structure. *GaSb* is 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 indirect bandgap. 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 [4]. Subjecting *GaSb* to high pressure leads to pressure induced metallization, structural phase transition and superconducting transition.

Wang et al [5] 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 *GaSb*[6-8]. This motivated us to take up the present

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investigation. 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 this compound [2]. We have analyzed the phenomena of metallization under high pressure of this material. 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 and metallization 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 and density of states calculations were performed for *GaSb* corresponding to different reduced volumes in *ZnS, NaCl* and *CsCl* structures, by the first-principle FP-LMTO method with in generalized gradient approximation (GGA). The details of the FP-LMTO method are well described in the literature[2] and we give here only the calculational details [1,3]. The electronic configurations of *Ga* and *Sb* are [Ar] $4s^2$ $4p^1$ $3d^{10}$ (Z = 31) and [Kr] $5s^2$ $5p^3$ (Z = 51) respectively. The valence electronic configurations chosen in our calculations are $4s^2$ $4p^1$ for *Ga*, $5s^2$ $5p^3$ for *Sb*. There are 8 valence electrons contributing to the valence bands. The final energy convergence is within 10^{-5} Ry. The calculated total energies were fitted to Murnaghan's equation of state (EOS), to determine the ground-state properties[6].

2.2 Band structure of GaSb under pressure

The band structures of *GaSb* were computed for various reduced volumes ranging from V/V_o=1.0 to 0.3 in steps of 0.05. Even though we have obtained the band structure for V/V_o values from 1.0 to 0.3, we have presented here the band structures of *GaSb* along the symmetry directions *Γ-X-W-L-Γ-K* and the corresponding density of states of *GaSb* (Figs.1 to 4). The volume compressions corresponding to V/V_o=1.0 and V/V_o=0.79 for *GaSb* only given. A single band nearer to the bottom arises from $5s^2$ electrons of *Sb* (Fig.1). The three bands appearing below the Fermi level are due to the $4s^2$, $4p^1$ electrons of *Ga* and $5p^3$ electrons of *Sb* (Fig.1). The empty conduction bands above the Fermi level are due to 4p, 4d states of *Ga* and 5d, 5p states of *Sb* (Fig.1). At normal pressure, the band gap of *GaSb* is indirect with valence band maximum at *Γ* point and conduction band minimum at *X* point with band gap value 0.726 eV. The calculated energy gaps are in agreement with the experimental value of 0.73 eV (Table 1)[4]. As pressure increases the width of the valence band and the empty conduction band get widened[7]. These changes leads to the narrowing of the band gap under pressure (Fig. 3).

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 *GaSb* corresponding to normal pressure is shown in Fig.2. At normal pressure the levels arising from $4s^2$ electrons of *Ga* give the long spike near the origin. The short spikes near the Fermi energy are due to $5s^2$, $5p^3$ electrons of *Sb* and $4p^1$ electron of *Ga*. The short peaks above the Fermi energy E_F are due to the 4p, 4d states of *Ga*and 5d, 5p states of *Sb*. The general features of the band structure and density of states (Figs 1-4) are similar to that of the group II-IV compounds [3].

3 Results and discussion

3.1 Ground state properties

The ground state properties and structural phase transitions are studied from the 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 *GaSb[1]*. 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

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$P = 1.5B_o [(V_o/V)^{7/3} - (V_o/V)^{5/3}] [1 + 0.75 (B_o^1 - 4) \{(V_o/V)^{2/3}-1\}]$ (1) to obtain the equilibrium lattice constant and other ground state properties. The relation between reduced volume and lattice constant is shown in Fig.5. Here lattice constant decreases with decrease of reduced volume. The relation between reduced volume and pressure is shown in Fig.6. When reduced volume decreases pressure increases[8].

In Table 1, the equilibrium lattice constant (a_o), band gap (E_g), bulk modulus (B_o) and its pressure derivative (B_o^1) values are compared with experimental [4] and previous theoretical works [5]. 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 [1].

3.2 Metallization

At normal pressure *GaSb* is a semiconductor. 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 *GaSb* are shown in Figs. 3 and 4 respectively. In *GaSb,* 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 *GaSb* is V/V_o=0.79 (*ZnS* structure), which corresponds to the pressure P_M = 5.4 GPa. At the metallization pressure, 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 *GaSb* (Fig.4). Thereafter $N(E_F)$ increases slowly with pressure and becomes fairly large at a particular value of V/V_o. The values of E_F and $N(E_F)$ corresponding to different V/V_o are used in studying the pressure variation of superconducting transition temperature. However, there are no experimental or theoretical study available for comparison at these pressures.

4. Conclusion

In the present investigation, the pressure dependent band structures and density of states of *GaSb* is computed and the results are used to study the metallization 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 *GaSb* (metallization).

Table 1. Equilibrium lattice constant (a_o), bulk modulus (B_o) and its pressure derivative (B_o^1) of *GaSb* in *ZnS* structure

Ground State Properties	GaSb		
	Present work	Experimental works [4]	Previous theoretical work[5]
a_o a.u.	11.5236	11.6	10.67
B_o Mbar	0.560	0.580	0.52
B_o^1	4.662	4.7	4.276
E_g eV	0.726	0.73	0.65

Table 2. Metallization pressure and metallization reduced volume in *GaSb*

Gallium Compound	Metallization	
	P_M GPa	$(V/V_o)_M$
GaSb	5.4	0.79

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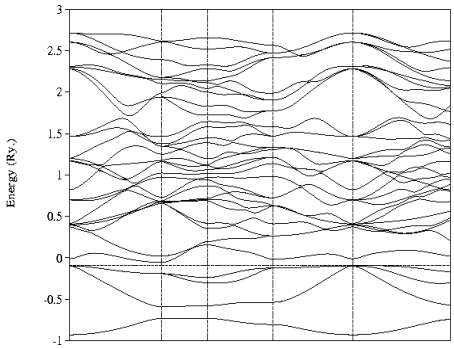

Fig.1 Band structure of GaSb at V/Vo=1 in zinc blend structure (normalpressure)

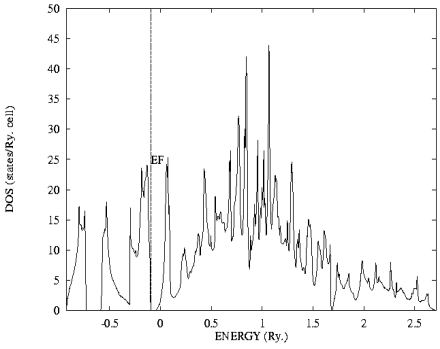

Fig.2 Density of states of GaSb at V/Vo=1 in zinc blende structure (normal pressure)

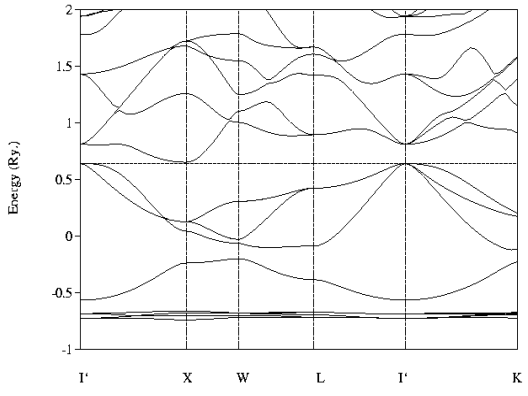

Fig.3 Band structure of GaSb at V/Vo=0.79 in ZnS structure (pressure = 5.4 GPa)

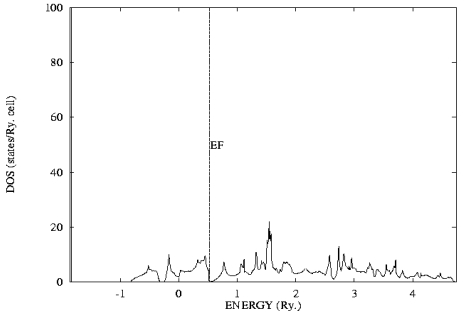

Fig.4 Density of states of GaSb at V/Vo=0.79 in ZnS structure (pressure = 5.4 GPa)

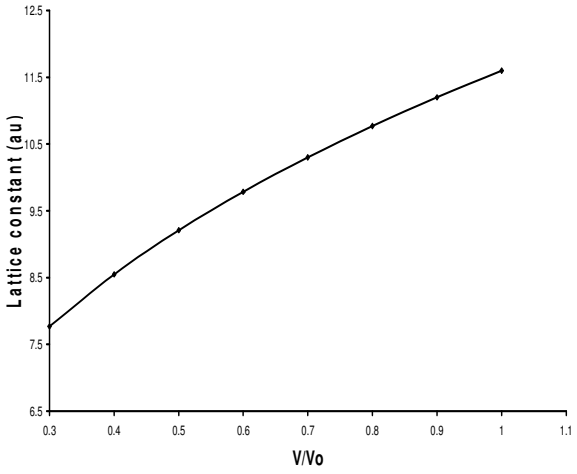

Fig.5. Relation between reduced volume and lattice constant

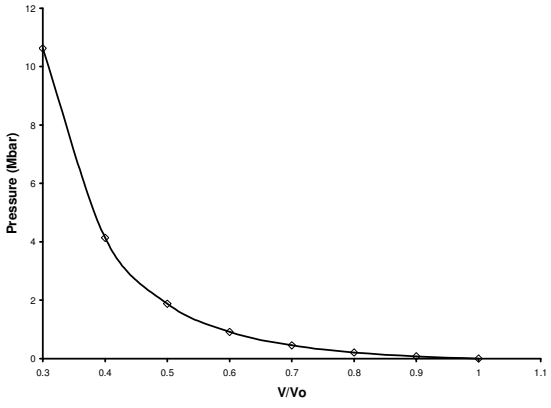

Fig.6. Relation between reduced volume and pressure

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