

Total energy, equation of state and bulk modulus of AlP, AlAs and AlSb semiconductors

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Abstract. Recently proposed model potential which combines both linear and quadratic types of interactions is employed for the investigation of some properties like the total energy, equation of state and bulk modulus of AlP, AlAs and AlSb semiconductor compounds using higher-order perturbation theory. The model potential parameter is determined using zero pressure condition. The ratio of the covalent bonding term E_{cov} to the second-order term E_2 is 6.77% to 11.85% which shows that contribution from higher order terms are important for zinc-blende-type crystals. The calculated numerical results of the total energy, energy band gap at Jones-zone face and bulk modulus of these compounds are in good agreement with the experimental data and found much better than other such theoretical findings. We have also studied pressure–volume relations of these compounds. The present study is carried out using six different screening functions along with latest screening function proposed by Sarkar *et al.* It is found from the present study that effect of exchange and correlation is clearly distinguishable.

Keywords. Pseudopotential method; semiconductor compounds; total energy; equation of state; bulk modulus.

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1. Introduction

It is difficult to compute static and dynamical properties of crystals such as cohesive energy, bulk modulus and lattice vibrations using information obtained from the band structure calculations. A pseudopotential perturbation approach is an effective technique for obtaining the various crystal properties without doing band calculations. The second-order perturbation theory based on the pseudopotential formalism has failed for covalent crystals mainly due to the large pseudopotential in these crystals and the energy gap on the Jones-zone face corresponding to the Fermi surface [1,2]. These facts are associated with covalent bonding character of these crystals. This character comes from higher than second-order terms and has an important role for the stability of lattices of the crystals having the diamond structure. In the second-order pseudopotential theory the crystals are unstable for shear distortion and the phonon dispersion curves show imaginary frequencies in

the transverse acoustic mode [3]. Bennemann [4] has tried an extension of pseudopotential theory by the t-matrix method to discuss the covalent bonds in covalent crystals, which is quite a laborious method.

To overcome all these problems pertaining to covalent crystal, Morita *et al* [5] have developed the perturbation theory for covalent crystals in terms of pseudopotential by taking into account the higher order terms corresponding to the covalent bonding effect using isotropic energy gap model. Soma [6–8] was successful in computing total energy and bulk modulus of some covalent compounds on the basis of extended perturbation theory. He has used historical model potentials like Ashcroft's empty core model potential [9] and local Heine–Abarenkov model potential [10] with an additional parameter to ensure minimum energy condition. Ito [11] has also reported the study of AlSb, GaSb and GaAs using local Heine–Abarenkov model potential [10] with self-consistent method to determine the model potential parameter.

Recently, we have proposed a model potential [12] which has been successfully applied to calculate some static properties of Si and Ge and same is used, in the present paper to investigate electronic properties of AlP, AlAs and AlSb semiconductors. The analytical form of our model potential [12] is given by

$$\begin{aligned} W_i(r) &= -\frac{Z_i e^2}{R_c^i} \left[\frac{3r}{2R_c^i} - \frac{r^2}{2(R_c^i)^2} \right], \quad r < R_c^i \\ &= -\frac{Z_i e^2}{r}, \quad r \geq R_c^i \end{aligned} \quad (1)$$

and momentum-space representation of our model potential is given by

$$W_{ib}(q) = -\frac{12\pi Z_i e^2}{\Omega q^3 R_c^i} \left[\frac{\sin(qR_c^i)}{2} - \frac{1}{qR_c^i} + \frac{\sin(qR_c^i)}{(qR_c^i)^2} \right], \quad (2)$$

where suffix *i* is 1 (for Al) or 2 (for P, As or Sb), Z_i is the ion valency, e is the electronic charge, Ω is the atomic volume and q is the wave vector. The value of model parameter is determined by satisfying zero pressure condition.

2. Method of computations

For a covalent crystal with diamond or zinc-blende structure based on the higher order perturbation theory, the total energy per atom of the crystal [5,6,12] is given by

$$E = E_i + E_0 + E_1 + E_2 + E_{cov}, \quad (3)$$

where E_i is the electrostatic energy of point ions immersed in the uniform gas of valence electrons, called the Madelung energy, E_0 is the sum of the kinetic, exchange and correlation energies of the valence electron, E_1 is the first-order perturbation energy of the valence electron due to the pseudopotential, E_2 is the second-order term and E_{cov} is the covalent correction term.

For the incorporation of exchange and correlation effects to the dielectric function, we have adopted seven approximations: Hartree (H) [13], Hubbard (HB) [14],

Table 1. The ratio of covalent bonding term E_{cov} to second-order term E_2 (%).

Compound	Present						Other [6]
	H	HB	K	VS	T	SS	
AlP	6.77	9.07	8.85	8.96	9.22	8.02	–
AlAs	7.02	9.66	9.49	9.64	10.01	8.65	–
AlSb	7.18	9.57	9.42	11.85	7.86	10.32	9.02–10.73

Table 2. The band gap E_g^x at the point x on the Jones-zone face (in eV).

Compound	Present	Other [6]	Observed [6]
AlP	3.73	–	–
AlAs	3.57	–	–
AlSb	3.22	3.59	4.2

Kleinman (K) [15], Kleinman and Langreth (KL) [15,16], Vashistha and Singwi (VS) [17], Taylor (T) [18], and Sarkar *et al* (SS) [19].

3. Results of calculations and discussion

Table 1 shows the spread of ratio of the covalent bonding term E_{cov} to the second-order term E_2 for different screening functions. In the present study, the spread of ratio E_{cov}/E_2 varies from 6.77 to 11.85% of the second-order term. The range of the ratio E_{cov}/E_2 for AlSb reported by Soma [6] is 9.02–10.73%. Thus we may conclude that in the zinc-blende-type crystals contributions from higher order terms are important.

The presently investigated band gap E_g^x of compounds at the Jones-zone face are tabulated in table 2 along with other available theoretical and observed data. The value of E_g^x for AlSb reported by Soma [6] is 4.96 eV which is incorrect. This is because he [6] obtained this result using the improper values of pseudopotential Fourier components which were reported for comparison of his data. It is obtained 3.59 eV for AlSb using data reported from his calculations.

Table 3 shows the total energy of AlP, AlAs and AlSb semiconductor compounds obtained by eq. (3) along with experimental and other reported values [6,8,20,21]. It is found from table 3 that the effect of exchange and correlation is clearly distinguishable. The percentage of deviation is within 1% when we use HB and K local-field correction functions for AlP. Excellent results are also obtained when we incorporate HB and VS in the case of AlAs and HB only in the case of AlSb. The total energy obtained with the exclusion of local field correction function deviates 8.45% for AlP, 9.43% for AlAs and 8.45% for AlSb from the experimental value. The maximum deviation in the total energy obtained with the incorporation of local field correction function to the dielectric function from the experimental

Table 3. The total energy E (in Ryd) per electron of AlP, AlAs and AlSb semiconductor compounds.

Compound	Present						Observed [6]	Others [6,8,20,21]	
	H	HB	K	VS	T	SS			
AlP								2.165	
								1.425	2.162
	2.0107	2.2018	2.1794	2.2215	2.248	2.1656	2.1963	2.1	2.190
									2.186
									2.196
AlAs								2.087	
								2.05	2.085
	1.9299	2.1148	2.0913	2.1354	2.159	2.0808	2.1308	2.05	2.113
								1.225	2.111
									2.122
AlSb								2.131	
								1.953	1.910
	1.7716	1.9387	1.9138	1.9605	1.9769	1.9099	1.935–1.939	1.976	1.937
								1.978	1.940
								1.990	1.955
							1.0	1.650	

value is 2.35% for AlP, 2.16% for AlAs and 2.16% for AlSb while the maximum deviation of the total energy reported by others [6,8,20,21] is 35.11% for AlP, 42.5% for AlAs and 48.37% for AlSb from the observed values. Thus numerical results of total energy of AlP, AlAs and AlSb using our model potential by incorporating different screening functions give excellent agreement with the experimental result and superior to other reported results.

Figures 1 to 3 show the pressure–volume relations for AlP, AlAs and AlSb. The present finding of equation of states with various local field correction functions for AlP, AlAs and AlSb at different volume are within the value obtained by inclusion of H and T local field correction to the dielectric function. Hence to avoid complication in the figures, equation of states obtained due to H and T are plotted. It is clear from figures 1 to 3 that the presently investigated pressure obtained by higher order perturbation theory agrees well with the pressure obtained by universal equation of state [22] for AlP, AlAs and AlSb semiconductors. Since the experimental data of equation of state of AlP, AlAs and AlSb are not available for comparison, these may be considered predictive for future reference.

The presently investigated bulk modulus (B) of AlP, AlAs and AlSb semiconductor compounds are tabulated in table 4 along with other theoretical and observed data [6,8,20,21]. From table 4, it is noticed that the deviation of our results of bulk modulus obtained with the use of screening function from observed values is 0.082–10.7% for AlP, 1.04–10.19% for AlAs and 2.05–6.11% for AlSb. The bulk modulus obtained with the use of H screening function deviate 32.9% for AlP, 34.9% for

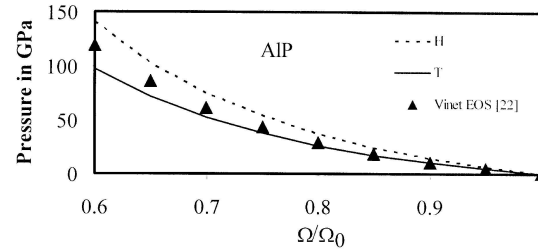


Figure 1. The pressure–volume relation of AlP.

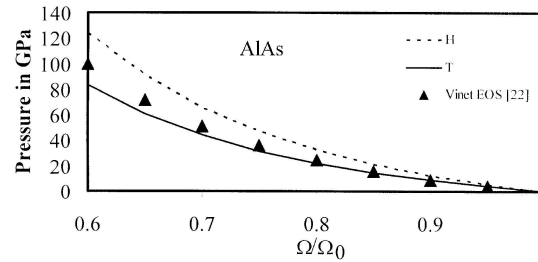


Figure 2. The pressure–volume relation of AlAs.

Table 4. The bulk modulus B (in 10^{12} dyn cm^{-2}) of AlP, AlAs and AlSb semiconductors compounds.

Compound	Present						Observed [6]	Others [6,8,20,21]	
	H	HB	K	VS	T	SS			
AlP	1.1496	0.8953	0.8964	0.8367	0.8149	0.8657	0.865	0.96	1.095
								0.984	1.057
								0.929	1.025
								0.997	0.984
								0.973	0.929
AlAs	0.9999	0.7546	0.7595	0.6999	0.681	0.7333	0.741	0.86	0.941
								0.79	0.887
								0.837	0.837
								0.702	0.702
								0.675	0.675
AlSb	0.7546	0.5339	0.5465	0.4873	0.4756	0.5256	0.593	0.58	0.667
								0.611	0.611
								0.58	0.58

AlAs and 46.5% for AlSb from the observed value. These results clearly indicate significance of the exchange and correlation effects through screening function. The results due to others [6,8,20,21] include the deviation ranging from 7.39 to 26.58%

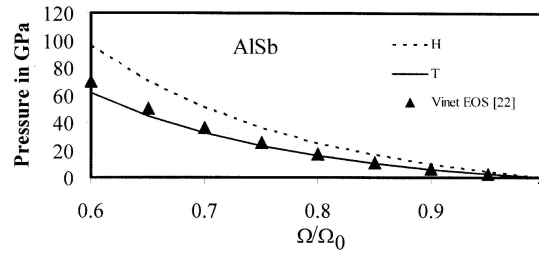


Figure 3. The pressure–volume relation of AlSb.

for AlP, 6.61 to 34.55% for AlAs and 2.19 to 18.38% for AlSb from the observed values. In comparison with the other theoretical results [6,8,20,21] the present findings are found much better.

Finally, we conclude while stating that the covalent correction terms are needed for proper explanation of electronic theory of tetrahedrally covalent semiconductors. In addition to this, the exchange and correlation effects are also playing a vital role. The overall superiority of present findings in explaining electronic properties of tetrahedrally covalent semiconductors confirms the application of our model potential, fruitfully.

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