Prediction of some mechanical and vibrational properties of GaX (X = P, As, Sb) semiconductor compounds

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Abstract

The static elastic constants (C_{11}, C_{12} and C_{44}), pressure derivative of elastic constants, pressure derivative of bulk modulus, propagation velocities of longitudinal and transverse waves in [100], [110] and [111] directions and Young modulus are investigated through computations using the higher-order perturbation theory based on pseudopotential formalism, in which we have applied our own proposed model potential for GaP, GaAs and GaSb semiconductor compounds. In the present calculations, two local-field correction functions are employed to consider exchange and correlation effects. The numerical values of the aforesaid properties are found to be sensitive to the selection of the local-field correction function and showing a significant variation with the change in the function. The presently investigated numerical data is found to have, in general, good agreement with the available experiment data and other such theoretical values.

Key Words: Semiconductor compound, pseudopotential method, elastic constant, pressure derivative of bulk modulus, pressure derivative of elastic constants

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1. Introduction

During last few years, much attention has been given towards the study of Group A^{III}B^{V} semiconductor compounds, for their potential applications in a variety of optoelectronic devices such as light emitting diodes, photovoltaic cells, photo detectors, lasers, modulators, integrated circuits, filters etc. Therefore, the experimental and theoretical study of physical properties of such materials is important and essential [1–8].

To investigate certain physical properties theoretically, previously we exploited successfully the higher-order perturbation theory to covalent crystals of Group IV elemental semiconductors, Group III-V semiconductor compounds, Group II-VI semiconductor compounds and solid solutions [9–13]. In the present work we have employed such theory together with the application of potential proposed by Jivani et al [9–13] for the

investigations of static elastic constants, pressure derivative of bulk modulus, pressure derivative of elastic constants, phonon related properties such as propagation velocities of longitudinal and transverse waves in [100], [110] and [111] directions and Young Modulus of GaP, GaAs and GaSb semiconductor compounds. Numerical results thus obtained are compared with available experiment data and other such theoretical findings. In the present investigation, the local-field correction functions due to Hartree (H) [14] and Farid et al (F) [15] are incorporated to see the impact of exchange and correlation effects.

2. Formulation of the problem

2.1. Model potential

The potential proposed by Jivani et al [9-13] is employed to describe electron-ion interactions in the present investigation. The analytical form of the potential in real space is

$$
\begin{aligned}
W(r) &= -\frac{Z\,e^2}{R_C^2}\left[\frac{3r}{2} - \frac{r^2}{2\,R_C}\right], & r < R_C, \\
&= -\frac{Z\,e^2}{r}, & r \geq R_C.
\end{aligned}
\tag{1}
$$

In equation (1), Z is the valency, e is the electronic charge and R_C is the parameter of the potential. This potential is sum of two terms within core: the first term varies linearly (attractive) with r, and the second term varies quadratically (repulsive) with r. The potential within the core is weak due to cancellation of repulsive and an attractive contribution. Hence, it is assumed that the potential within the core should be neither zero nor constant, but it should vary as a function of r. The potential outside the core is Coulombian in nature. Thus, the potential has the novel feature of representing varying cancellation of potential within the core and it is continuous at core.

The form factor $W(q)$ of the potential in wavenumber space is

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

Here, Ω is the atomic volume and q is wave vector. The value of parameter of the potential R_C is determined by fitting with the experimental value of the bulk modulus of the semiconductor compound under investigation [12–13].

In equation (2), the screening function $\varepsilon(q)$, which takes into account the conduction electrons interactions, is of the form

$$
\varepsilon(q) = 1 + \{\varepsilon_H(q) - 1\}\{1 - f(q)\}.
\tag{3}
$$

In this expression $\varepsilon_H(q)$ is the static Hartree dielectric function and $f(q)$ is the correlation function for the exchange and correlation motion of the conduction electrons.

In the present study, Hartree local-field correction function (without screening function) [14], along with screening function proposed by Farid et al (with screening function) [15], is used to consider exchange and correlation effects to the dielectric function. The H-screening function [14] is purely static, i. e.

$$
f(q) = 0.
\tag{4}
$$

Thus, it does not include the exchange and correlation effects and hence it becomes a Hartree screening function [14], to judge the effect of absence of any such function in the present investigations.

The Farid et al local-field correction function [15] is a fitting formula, derived for the dielectric screening function of the degenerate electron liquids at metallic and lower densities. It satisfies the self consistency condition in the compressibility sum rule and short range correlations. Farid et al local-field correction function [15] is chosen to see the effect of presence of the same in the present investigations. The mathematical expression of Farid et al local-field correction function can be found detailed in reference [15].

2.2. Total energy calculation

Under the higher-order perturbation theory, the total energy per atom of the covalent crystal [9-13] can be expressed as

$$E = E_i + E_0 + E_1 + E_2 + E_{Cov}. \tag{5}$$

In equation (5), 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 is the first-order perturbation energy of the valence electron due to the pseudopotential; E_2 is the second-order term or band structure energy; and E_{Cov} is the covalent correction term to the total energy. The covalent correction term E_{Cov} is approximately equal to sum of third and fourth-order perturbation energy to the total energy.

2.3. Static elastic constants

Elastic constants are related to the hardness of the materials, and provide valuable information to understand materials. Therefore, a detailed knowledge of the elastic properties is an important subject to study either for fundamental or applied consideration.

There are two methods to calculate the elastic constants, static method and dynamic method based on pseudopotential approach. In the static treatment, we consider a cubic crystal system consisting of ions located on the lattice points R_i and an electron gas composed of valence electrons.

There are three elastic constants of a cubic crystal which are obtained by considering the following homogeneous deformations [12]. First, consider uniform volume expansion denoted by $R'_{ix} = v^{\frac{1}{3}} R_{ix}$, $R'_{iy} = v^{\frac{1}{3}} R_{iy}$ and $R'_{iz} = v^{\frac{1}{3}} R_{iz}$. Then, the static bulk modulus is obtained by second-order differentiation of total energy E.

Next, considering shear deformation in one plane denoted by $R'_{ix} = R_{ix} + \gamma_1 R_{iy}$, $R'_{iy} = R_{iy}$ and $R'_{iz} = R_{iz}$, where crystal volume is maintained to be constant, shear modulus C_{44} is obtained. This deformation is also denoted by $G'_x = G_x$, $G'_y = G_y - \gamma_1 G_x$ and $G'_z = G_z$ in wave number space. In the higher-order perturbation, the static shear modulus C_{44} is given by only contribution through reciprocal lattice vectors G which is given by

$$C_{44} = \frac{1}{2\Omega} \sum_{G \neq 0} G_x^2 \frac{\partial^2 \phi(G)}{\partial G_y^2}, \tag{6}$$

where

$$\phi(G) = \frac{4\pi Z^2 e^2}{\Omega G^2} - \Omega \frac{W_b(G)^2}{\varepsilon(G)} \frac{\chi_0(G)}{1 - 4\pi e^2 f(G)\chi_0(G)/G^2} - \frac{n(E_F)}{6} \left\{ |W_{eff}(G)|^2 - |W(G)|^2 \right\} \delta_{G,\{220\}}. \tag{7}$$

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Lastly, considering compression in one direction by $R'_{ix} = (1 + \varepsilon_1)R_{ix}$, $R'_{iy} = R_{iy}/(1 - \varepsilon_1)$ and $R'_{iz} = R_{iz}$, where crystal volume is also maintained to be constant, shear modulus $C' = (C_{11} - C_{12})/2$ is obtained. This deformation is also denoted by $G'_x = G_x/(1 + \varepsilon_1)$, $G'_y = G_y(1 + \varepsilon_1)$ and $G'_z = G_z$ in wave number space. The static shear modulus C' is given by

$$C' = \frac{1}{4\,\Omega} \sum_{G \neq 0} \left[G_x^2 \frac{\partial^2 \phi\,(G)}{\partial\, G_x^2} + G_y^2 \frac{\partial^2\, \phi\,(G)}{\partial\, G_y^2} - 2G_x G_y \frac{\partial^2\, \phi\,(G)}{\partial\, G_x\, \partial G_y} \right]. \tag{8}$$

The elastic constants C_{11} and C_{12} are obtained by using the following relations:

$$C' = (C_{11} - C_{12})/2 \text{ and} \tag{9}$$

$$B = (C_{11} + 2\,C_{12})/3. \tag{10}$$

2.4. Pressure derivative of bulk modulus and elastic constants

The pressure derivatives of the elastic stiffness constants $\frac{d\,C_i}{dP}$ ($C_i = B$, C_{44} and C') at low temperatures are given by

$$C'_i = \frac{d\,C_i}{dP} = -\left(\frac{\Omega}{B} \frac{d\,C_i}{d\,\Omega} \right). \tag{11}$$

2.5. Poisson's ratio

Poisson's ratio σ is determined as [16]

$$\sigma = \frac{C_{12}}{(C_{11} - C_{12})}. \tag{12}$$

2.6. Young's modulus

From the calculated values of the bulk modulus and Poisson's ratio, Young's modulus (Y) is derived as [16]

$$Y = 3\,B\,(1 - 2\sigma). \tag{13}$$

2.7. Acoustic wave speeds

In the cubic system the propagation velocity of longitudinal waves in [100], [110] and [111] directions is given as [16–17]:

$$v_L\,[100] = \left[\frac{C_{11}}{\rho} \right]^{\frac{1}{2}}, \tag{14}$$

$$v_L\,[110] = \left[\frac{C_{11} + C_{12} + 2\,C_{44}}{2\,\rho} \right]^{\frac{1}{2}}, \tag{15}$$

$$v_L\,[111] = \left[\frac{C_{11} + 2\,C_{12} + 4\,C_{44}}{3\,\rho} \right]^{\frac{1}{2}}. \tag{16}$$

The propagation velocity in the transverse mode is expressed by

$$v_T[100] = v_{T_1}[110] = \left[\frac{C_{44}}{\rho}\right]^{\frac{1}{2}}, \tag{17}$$

$$v_T[110] = \left[\frac{C_{11} - C_{12}}{2\rho}\right]^{\frac{1}{2}}, \tag{18}$$

$$v_T[111] = \left[\frac{C_{11} - C_{12} + 2C_{44}}{3\rho}\right]^{\frac{1}{2}}. \tag{19}$$

3. Results and discussion

3.1. Static elastic constants

The elastic constants resulting from higher-order perturbation theory are summarized in Tables 1 to 3 for GaP, GaAs and GaSb semiconductor compounds, respectively. The highest values of elastic constants (C_{11}, C_{12} and C_{44}) are obtained in the case of GaP semiconductor compound, and the lowest such values are observed in the case of GaSb semiconductor compound. This is due to extreme difference in atomic volume among the three semiconductors. Thus, the values of elastic constants, C_{11}, C_{12} and C_{44}, depend on atomic volume of the compound, and increase with the volume of semiconductor compounds.

Table 1. Static elastic constants (in GPa) for GaP semiconductor compound.

Elastic Constants	Present results with different f(q)		Experiment [1, 4, 18]	Other calculations [1, 4, 18]
	H [14]	F [15]		
C_{11}	176.4	147.3	140.5, 141.2	129, 140, 140.5, 140.8, 145, 147, 150.7, 178.8, 203
C_{12}	44.9	59.6	62.03, 62.53	56.3, 57.8, 61.0, 61.6, 61.8, 62.0, 62.03, 62.8, 62.92, 65.7, 142
C_{44}	92.2	78.3	70.33, 70.47	51.2, 55.6, 58.9, 68.5, 70.3, 76.3, 79.0, 81.66, 82.2, 130

Table 2. Static elastic constants (in GPa) for GaAs semiconductor compound.

Elastic Constants	Present results with different f(q)		Experiment [1, 18, 19]	Other calculations [1, 18, 19]
	H [14]	F [15]		
C_{11}	150.8	125.7	118.1, 122.3	116, 120, 122, 122.8, 123, 124.2, 125, 147.6, 168
C_{12}	36.8	49.6	53.2, 53.8, 57.1	46.0, 50.7, 50.9, 51.4, 53.0, 55.2, 119
C_{44}	83.6	72.9	59.2, 59.5, 60.0	42.4, 50.7, 52.8, 52.9, 57.8, 62.0, 63.4, 107

Table 3. Static elastic constants (in GPa) for GaSb semiconductor compound.

Elastic Constants	Present results with different f(q)		Experiment] [5, 18]	Other calculations [3, 5, 18]
	H [14]	F [15]		
C_{11}	112.4	94.7	88.34	78.48, 86.8, 88.4, 88.5, 89.4, 99.1, 92.7, 126.6
C_{12}	28.3	37.3	40.23	33.5, 34.47, 37.6, 38.7, 40.3, 44.1, 97
C_{44}	70.1	66.7	43.22	36.5, 38.98, 40.7, 43.2, 45.2, 46.2, 73.7

From Tables 1 and 3, it is noticed that the deviation of our result of elastic constants (C_{11}, C_{12} and C_{44}) from the observed values [1, 4–5, 18–19] is 3.9% to 31.1% for GaP, 6.4% to 39.3% for GaAs and 7.2% to 62.7% for GaSb semiconductor compounds. The results due to others [1, 3–5, 18, 19] include the deviation ranging from 8.2% to 128.9% for GaP, 1.8% to 123.7% for GaAs and 11.2% to 141.1% for GaSb from the observed values. It is also noticed that the numerical values of elastic constants obtained using Farid et al screening function [15] yield the deviation ranging from 3.9% to 7.2% for GaX and such numerical values obtained by using H local-field correction function [14] deviate 31.1% to 54.3% for GaX from the observed values [1, 4-5, 18–19].

Thus, from Tables 1 to 3, we can conclude that though the calculated values of elastic constants GaX scatter in a bit wide range around the observed values, present findings are an improvement over previously reported theoretical values [1, 3–5, 18, 19].

3.2. Pressure derivative of bulk modulus and elastic constants

The pressure derivative of the bulk modulus and elastic constants C_i' are presented in Tables 4 to 6 for three Gallium based Group III-V semiconductor compounds. From Tables 4 to 6, the calculated pressure derivative of bulk modulus is found to be about 4, which is consistent with universal theory of equation of state [23]. As per our knowledge, no experimental and theoretical results of some of the pressure derivatives of elastic constants (such as C_{11}' and C_{12}' of GaP and GaSb) the semiconductor compounds are reported so far. We think that the theoretical estimation is the only reasonable tool to obtain such important information. The present results of pressure derivative of elastic constants for these three binary compounds may be useful for comparison in future with theoretical as well as experimental research of such compounds.

Table 4. Pressure derivative of bulk modulus and elastic constants for GaP semiconductor compound.

C_i'	Present results with different f(q)		Experiment [8]	Other calculations [1, 2, 4, 6, 8, 20]
	H [14]	F [15]		
B'	4.54	4.03	4.5, 4.8	3.69, 3.68, 3.91, 4.27, 4.30, 4.339, 4.34, 4.40, 4.5, 4.60, 4.76
C_{11}'	6.02	4.86	-	3.7, 3.91, 4.33, 4.77, 5.0
C_{12}'	3.80	3.61	-	4.13, 4.28, 4.79, 4.9, 5.0
C_{44}'	1.22	0.77	1.137	0.6, 0.92, 1.1, 1.92, 3.20

Table 5. Pressure derivative of bulk modulus and elastic constants for GaAs semiconductor compound.

C_i'	Present results with different f(q)		Experiment	Other calculations
	H[14]	F [15]	[19, 21, 22]	[1, 19, 20-22]
B'	4.63	4.09	4.49, 4.56, 4.67	3.36, 3.94, 4.018, 4.02 4.49, 4.80, 5.24, 4.36 ∼ 4.71
C_{11}'	6.18	4.97	4.6	5.3
C_{12}'	3.86	3.66	4.6	5.1
C_{44}'	1.27	0.80	1.1, 1.2	0.977, 1.1, 1.36, 1.4, 2.4

Table 6. Pressure derivative of bulk modulus and elastic constants for GaSb semiconductor compound.

C_i'	Present results with different f(q)		Experiment	Other calculations
	H[14]	F[15]	[8,21]	[3, 20, 21]
B'	4.77	4.26	4.75, 4.78	3.71, 3.83, 4.44, 4.662, 4.90, 4.58 ∼ 5.01
C_{11}'	6.38	5.25	-	-
C_{12}'	3.97	3.77	-	-
C_{44}'	1.29	0.87	-	0.32, 1.0

3.3. The phonon related properties

Phonon related properties, such as Poisson's ratio, Young's modulus and propagation velocities of longitudinal and transverse waves in [100], [110] and [111] directions in elastic medium, are determined and displayed in Tables 7 to 9 for GaX (X = P, As and Sb) semiconductor compounds.

The theoretically investigated such values for GaP and GaAs semiconductor remarkably match with the available experimental values [18] and other reported such theoretical values [4, 5]. The experimental value of such physical quantities for GaSb semiconductor is not available and hence to compare our theoretical values, the theoretical results obtained by putting experimental values of (C_{11}, C_{12}, C_{44}) and B in equations (12–19), as shown in Table 9.

Table 7. The phonon related properties for GaP semiconductor compound.

Properties	Present results with different f(q)		Experiment	Other
	H[14]	F[15]	[18]	calculation [4]
σ	0.203	0.288	0.31	0.2296
$Y_{(GPa)}$	158.2	113.0	103.0	-
$v_L[100]_{(m/s)}$	5690	5201	5830	-
$v_L[110]_{(m/s)}$	6102	5777	6430	-
$v_L[111]_{(m/s)}$	6233	5956	6630	-
$v_T[100]_{(m/s)}$	4114	3791	4120	-
$v_{T_2}[110]_{(m/s)}$	3474	2837	3080	-
$v_T[111]_{(m/s)}$	4396	3866	3460	-

Table 8. The phonon related properties for GaAs semiconductor compound.

Properties	Present results with different f(q)		Experiment
	H[14]	F[15]	[18]
σ	0.196	0.283	0.31
$Y_{(GPa)}$	136.4	97.6	86.0
$v_L[100]_{(m/s)}$	5165	4715	4730
$v_L[110]_{(m/s)}$	5602	5328	5240
$v_L[111]_{(m/s)}$	5740	5517	5400
$v_T[100]_{(m/s)}$	3846	3590	3350
$v_{T_2}[110]_{(m/s)}$	3176	2594	3350
$v_T[111]_{(m/s)}$	4072	3616	2800

Table 9. The phonon related properties for GaSb semiconductor compound.

Properties	Present results with different f(q)		From Calculation	Other calculation [5]
	H[14]	F[15]		
σ	0.201	0.283	0.2296	0.239
$Y_{(GPa)}$	101.00	73.6	63.2	-
$v_L[100]_{(m/s)}$	4294	3942	3989	-
$v_L[110]_{3(m/s)}$	4800	4667	4400	-
$v_L[111]_{(m/s)}$	4.957	4.885	4.529	-
$v_T[100]_{(m/s)}$	3391	3309	2790	-
$v_{T_2}[110]_{(m/s)}$	2627	2170	2081	-
$v_T[111]_{(m/s)}$	3502	3231	2842	-

4. Conclusions

The following conclusions may be drawn from the present investigations.

(i) We have successfully reported certain elastic and vibrational properties of the GaX (X = P, As and Sb) semiconductor compounds such as elastic constants, pressure derivative of elastic constants, pressure derivative of bulk modulus, Poisson's ratio, Young's modulus, acoustic velocities, etc., using our own proposed model potential [9–13], without any additional adjustable parameters with the higher-order perturbation theory. Finally, we believe that, in spite of simplicity of this method, our potential has yielded good estimate for elastic properties of the Ga-based three Group III-V semiconductor compounds.

(ii) This work used for the first time the screening function proposed by Farid et al. [15]. The elastic constants and pressure derivative of bulk modulus and pressure derivative of elastic constants of the presently investigated physical quantities under investigations have been found to generate larger values with inclusion of the H [14] screening function than results due to Farid local-field correction function [15].

(iii) In most cases, the present results due to exclusion of the exchange and correlation effect [14] are found to deviate much more than the results due to inclusion of the Farid et al local- field correlation function [15]. In general, the incorporation of Farid et al local-field correlation function [15] yielded better results than those results due to H local-field correction function [14].

(vi) Results presented in this paper compare favorably with the available experimental information and other such theoretical calculations. Our present results provide a set of theoretical values of pressure derivative of bulk modulus and pressure derivative of elastic constants, which may be useful for future reference.

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