Effect of pressure on some optical properties of Ga\textsubscript{x}In\textsubscript{1-x}P semiconductors

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Abstract. A theoretical procedure is presented for the study of optical properties of ternary alloy Ga\textsubscript{x}In\textsubscript{1-x}P. The calculations are based on the pseudopotential formalism in which local potential coupled with the virtual crystal approximation (VCA) is applied to evaluate the effect of pressure on the optical properties like refractive index, electronic polarizability, plasmon energy, dielectric constant and equation of state for gallium concentration \(x = 0, 0.25, 0.50, 0.75\) and 1 of the ternary alloy Ga\textsubscript{x}In\textsubscript{1-x}P. To incorporate the screening effect, local field correction functions due to Hartree, Taylor, Ichimaru et al. and Nagy are employed. The refractive index, electronic polarizability and dielectric constant computed for the parent binary compounds GaP and InP are in satisfactory agreement with the experimental report. It is seen that the refractive index of Ga\textsubscript{x}In\textsubscript{1-x}P decreases nonlinearly with the increase in pressure. The results obtained using Hartree’s screening functions are not very close to the experimental data as it does not include any exchange and correlation effects. Overall good agreement with the experimental and other theoretical findings confirms the application.

1. Introduction
Recently there has been increasing interest in the group II-VI and III-V semiconductor ternary alloys as their lattice parameter and energy band gap can be changed and fabricated independently, which make them suitable materials for optical spectroscopy, optoelectronic applications. Group III-V compounds are suitable to fabricate light emitting diodes, infrared detectors and infrared diode lasers, high speed switching devices and communication devices such as emitters, wave guides in the infrared to visible region \[1-2\]. Ternary alloy Ga\textsubscript{x}In\textsubscript{1-x}P has wide applications in high-power and high-frequency electronics. It is used mainly in high electron mobility transistor (HEMT) \[3\], heterojunction bipolar transistor (HBT) \[4-6\], for the fabrication of high efficiency solar cells used for space applications \[7-8\]. Ga\textsubscript{0.5}In\textsubscript{0.5}P which is almost lattice matched to GaAs; is used as vertical cavity surface emitting lasers (VCSELS) for plastic optical fibers \[9\]. These ternary alloys are very sensitive to external influence such as temperature, external fields and strains, which make them strong candidates for sensors \[10\]. A very small change in the pressure gives noticeable change in their optoelectronic properties. Therefore the study of the variation of optical properties as a function of pressure is very important in the fabrication or tailoring of different optical devices. In the present paper, we have studied the effect of pressure on the optical properties like refractive index, electronic polarizability and dielectric constant along with some physical properties like total energy, static bulk
modulus and plasmon energy for different gallium concentration \(x = 0, 0.25, 0.50, 0.75\) and 1.0 for the ternary alloy \(\text{Ga}_x\text{In}_{1-x}\text{P}\) using pseudopotential theory beyond second order with our well established single parametric model potential and modified virtual crystal approximation (VCA) [11]. We have used Nagy’s static local field correction function (N) [12] to include exchange and correlation effects. The results are compared with those obtained using local field correction functions due to Hartree (H) [13], Taylor (T) [14] and Ichimaru and Utsumi (IU) [15].

The paper is organized as follows. In section 1 we give a brief introduction. Section 2 contains a theoretical background for the calculation procedure. Section 3 covers discussion of the results. A summary of our conclusions is narrated in the section 4.

2. Theory

The bare-ion potential used in the present investigations is proposed in r-space [10-11] is

\[
W^{\text{ion}}(r) = \frac{Z e^2}{2R_c} \left[ 2 - \left( \frac{r}{R_c} \right)^2 \exp\left( -\frac{r}{R_c} \right) \right] \text{ for } r \leq R_c
\]

\[
W^{\text{ion}}(r) = -\frac{Z e^2}{r} \text{ for } r \geq R_c
\]

Here \(Z\), \(e\) and \(R_c\) are valency, electronic charge and pseudo core radius respectively. Here \(R_c\) is estimated through zero pressure condition.

It is to be noted that to represent core-core repulsion usually Born-Mayer term is employed. We have also incorporated this feature in our potential through exponential factor. Inside the core, it is represented as the combination of linear and quadratic terms modulated by repulsive exponential factor, which tends to cancel Coulomb potential inside the core. While outside the core, it has the Coulombian tail. It becomes analytic at \(r = 0\), and smoothness of the bare-ion potential due to exponential term results in to faster conversions in r-space. In addition this bare-ion potential is continuous at the core.

To incorporate the exchange and correlation effects in the dielectric function, Nagy’s static local field correction function [12] is used. It is given by,

\[
f(q)=1 - g(0, n) + \frac{c b}{c^2 + q^2} - \frac{g(0, n)}{q} \tan^{-1} \frac{q}{c}
\]

In equation (3), ‘\(q\)’ is a reciprocal lattice vector, ‘\(g(0, n)\)’ (i.e. \(g(r, n)\)) is the density dependent pair-correlation function. The detailed expressions of form factor and Nagy’s screening function (N) [12] are given elsewhere [10, 16]. The local field correction functions proposed by H [13], T [14] and IU [15] are also employed for comparative study with Nagy’s screening function (N) [12].

Table 1. Input parameters.

| Compound | Structure | Atomic Volume (a.u.³) |
|----------|-----------|-----------------------|
| GaP      | Zinc-blende | 136.70                |
| InP      | Zinc-blende | 170.50                |

3. Results and Discussion

The crystal energy per electron and bulk modulus computed for the different gallium concentration \(x = 0, 0.25, 0.50, 0.75\) and 1.0 of ternary semiconductor \(\text{Ga}_x\text{In}_{1-x}\text{P}\) using N [12], H [13], T [14] and IU [15] along with the experimental findings are shown in table 2. It is seen that H [13] produced higher values of energy and bulk modulus while IU [15] produced lower values energy and bulk modulus in all four screening functions. As H [13] does not include any exchange and correlation effects, it suggests that inclusion of exchange and correlation effect is essential for energy calculations and related properties. The total energy and bulk modulus computed for GaP by N [12] are found in good agreement with the experimental data cited in [17]. While some deviation is observed for InP.
Table 2. Total crystal energy and bulk modulus of Ga$_x$In$_{1-x}$P.

| Material   | -E$_T$ (Ryd / electron) | B (GPa) |
|------------|-------------------------|---------|
|            | N [12] | H [13] | T [14] | IU [15] | Exp. [17] | N [12] | H [13] | T [14] | IU [15] | Exp. [17] |
| InP        | 2.07   | 1.86   | 2.08   | 2.15   | 2.18   | 60.7    | 87.9   | 57.9   | 52.5   | 71.0,72.5 |
| Ga$_{0.25}$In$_{0.75}$P | 2.12   | 1.90   | 2.12   | 2.20   |        | 67.3    | 93.8   | 64.0   | 59.0   | -         |
| Ga$_{0.50}$In$_{0.50}$P | 2.16   | 1.93   | 2.17   | 2.23   |        | 74.2    | 100.8  | 70.5   | 65.6   | -         |
| Ga$_{0.75}$In$_{0.25}$P | 2.20   | 1.97   | 2.21   | 2.28   |        | 80.5    | 108.0  | 76.5   | 71.6   | -         |
| GaP        | 2.24   | 2.01   | 2.25   | 2.32   | 2.22   | 85.6    | 115.0  | 81.3   | 76.3   | 88.7      |

The refractive index (n) computed using relation of Reddy and Ahammed [18] alongwith other theoretical and experimental results [19-21] for different gallium concentration x of ternary alloy Ga$_x$In$_{1-x}$P are shown in table 3. The present refractive index values can be utilized to evaluate electronic polarizability ($\alpha_{pol}$) by using Lorentz-Lorentz formula [20] for different gallium concentration x of ternary alloy Ga$_x$In$_{1-x}$P are also shown in table 3. It is seen that the refractive index and electronic polarizability computed using present approach for GaP are in satisfactory agreement with the experimental results [20] and found in the range of other such theoretical predicted data [21-22]. Some overestimation is observed for InP. The results obtained using N [12] are quite close to the experimental results compared to other screening functions. A large deviation observed in the results computed by H [13] is due to absence of exchange and correlation terms in it.

Table 3. Refractive index and electronic polarizability ($10^{-24}$ cm$^3$) for Ga$_x$In$_{1-x}$P.

| Material   | n | $\alpha_{pol}$ |
|------------|---|----------------|
|            | N [12] | H [13] | T [14] | IU [15] | Exp. [20] | Others [19,21] | N [12] | H [13] | T [14] | IU [15] | Exp. [20] | Others [19,21] |
| InP        | 3.30 | 2.78   | 3.37   | 3.51   | 3.30   | 3.10,3.40 | 9.19  | 8.28   | 9.28   | 9.46   | 8.94      | 8.64,8.92     |
| Ga$_{0.25}$In$_{0.75}$P | 3.15 | 2.69   | 3.23   | 3.34   | -      | -         | 8.57  | 7.72   | 8.68   | 8.84   | -         | -             |
| Ga$_{0.50}$In$_{0.50}$P | 3.01 | 2.59   | 3.09   | 3.19   | -      | -         | 7.94  | 7.13   | 8.06   | 8.20   | -         | -             |
| Ga$_{0.75}$In$_{0.25}$P | 2.90 | 2.49   | 2.98   | 3.07   | -      | -         | 7.32  | 6.51   | 7.43   | 7.57   | -         | -             |
| GaP        | 2.82 | 2.40   | 2.89   | 2.98   | 2.90   | 2.96,3.23 | 6.71  | 5.90   | 6.83   | 6.96   | 6.87      | 6.74,6.85     |

The plasmon energy ($n\omega_p$) and high frequency dielectric constant ($\varepsilon_\infty$) computed for ternary semiconductor alloy Ga$_x$In$_{1-x}$P for gallium concentration x = 0, 0.25, 0.50, 0.75 and 1.0 are shown in table 4.

Table 4. The plasmon energy and high frequency dielectric constant for Ga$_x$In$_{1-x}$P.

| Material   | $n\omega_p$ | $\varepsilon_\infty$ |
|------------|-------------|----------------------|
|            | N [12] | H [13] | T [14] | IU [15] | Exp. [19] | Others [19] | N [12] | H [13] | T [14] | IU [15] | Exp. [19] | Others [19] |
| InP        | 14.9      | 17.9   | 14.5   | 13.8   | 14.8   | 16.0   | 11.1   | 8.2    | 11.4   | 12.0   | 10.9      | 11.3        |
| Ga$_{0.25}$In$_{0.75}$P | 15.6      | 18.5   | 15.3   | 14.6   | -      | -      | 10.3   | 7.7    | 10.7   | 11.3   | -         | -           |
| Ga$_{0.50}$In$_{0.50}$P | 16.4      | 19.1   | 16.0   | 15.4   | -      | -      | 9.6    | 7.1    | 10.0   | 10.5   | -         | -           |
| Ga$_{0.75}$In$_{0.25}$P | 17.1      | 19.9   | 16.7   | 16.1   | -      | -      | 9.0    | 6.4    | 9.4    | 9.9    | -         | -           |
| GaP        | 17.7      | 20.5   | 17.2   | 16.7   | 16.5   | 16.5   | 8.5    | 5.8    | 8.9    | 9.4    | 9.1       | 10.0        |

It is seen that the present results of the plasmon energy and high frequency dielectric constant are closely agree with the experimental and other such theoretical findings for GaP and InP.
The present results of refractive index as a function of pressure using screening functions due to Nagy [12] and Hartree [13] for different gallium concentrations $x$ of ternary semiconductor Ga$_{x}$In$_{1-x}$P are shown in figures 1 and 2, respectively.

![Figure 1](image1.png) Refractive index as a function of pressure using Nagy’s screening function for Ga$_{x}$In$_{1-x}$P.

![Figure 2](image2.png) Refractive index as a function of pressure using Hartree’s screening function for Ga$_{x}$In$_{1-x}$P.

It is seen that the refractive index of Ga$_{x}$In$_{1-x}$P decreases nonlinearly with the increase in pressure for all gallium concentrations. The present results of refractive index using Nagy [12] are in satisfactory agreement with the available experimental results at pressure $P = 0$ GPa. While some underestimation is observed for Hartree [13], this is due to absence of exchange and correlation effects in Hartree [13]. The noticeable difference is observed between results of refractive indices computed using Nagy [12] and Hartree [13] at zero pressure but this difference decreases with increase in pressure. To keep this paper in prescribe length; we discuss remaining properties with Nagy’s screening function [12] only. The pressure dependency of electronic polarizability and plasmon energy are shown in figure 3 and figure 4 respectively.

![Figure 3](image3.png) Electronic polarizability as a function of pressure using Nagy’s screening function for Ga$_{x}$In$_{1-x}$P.

![Figure 4](image4.png) Plasmon energy as a function of pressure using Nagy’s screening function for Ga$_{x}$In$_{1-x}$P.

It is seen that the electronic polarizability decreases and plasmon energy increases nonlinearly with increase in pressure, show same nature for all gallium concentration. It is also seen that the electronic polarizability decreases and plasmon energy increases with increase in gallium concentration. The literature survey reveals that there is no such theoretical work has been done so far earlier so we could not compare our results. The high frequency dielectric constant as a function of pressure is shown in figure 5. It shows same nonlinearity in nature. It decreases with increase in the gallium concentration. It is observed that the dielectric constant becomes negative for very high pressure (which is not shown in the figure 5).

The pressure–volume relationship (equation of states) for ternary semiconductor Ga$_{x}$In$_{1-x}$P is shown in figure 6. It is observed that pressure increases with increase in relative volume compression.
In the present study, we have considered compression up to 70%; which is now possible to achieve due to advancement in DAC techniques. It is seen that the pressure increase with the increase in the gallium concentration on the same relative volume compression. It is found that on 70% compression, the pressure reaches 18 GPa for InP ($x = 0$) and 24 GPa for GaP ($x = 1$). This characteristic suggests that ternary alloy Ga$_{1-x}$In$_x$P can be used with higher gallium concentration at the places where large variations in pressure have to be considered.

![Figure 5](image1.png)  
**Figure 5** High frequency dielectric constant as a function of pressure using Nagy’s screening function for Ga$_{1-x}$In$_x$P.

![Figure 6](image2.png)  
**Figure 6** Total pressure as a function of relative volume using Nagy’s screening function for Ga$_{1-x}$In$_x$P.

4. Conclusions

In the present investigation it is found that the total energy and bulk modulus computed for GaP and InP are matched with the experimental findings. The present findings of refractive index, electronic polarizability, plasmon energy and high frequency dielectric constant are found in good agreement with the experimental data and other such theoretical findings. It is seen that the refractive index, electronic polarizability and dielectric constant decrease nonlinearly with the increase in pressure while plasmon energy increases nonlinearly with the increase in the pressure. It is observed that all optical properties are noticeably changed with the gallium concentration. The predicted optical properties for different gallium concentrations for the ternary semiconductor Ga$_{1-x}$In$_x$P to the best of our knowledge; are reported for the first time in this paper, and we hope that the present findings will be considered as reference in future. Nagy’s static local field correction function [12] has been first time used in such study. Finally, we conclude that present results obtained using our novel model potential are satisfactory and could be used for further comprehensive study of such system of semiconductors.

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