ARYAVART SHODH VIKAS PATRIKA
RNI TITLED NO. UPBIL04292RNI
REG. NO. UPBIL/2014/66218 **PP. No.- 235-239**

I S S N NO. - 2347 – 2944 (Print)
e–I S S N NO.- 2582 – 2454 (Online)
Vol.-18, No.-III, Issues-33, YEAR-July-Sept. 2024

OPTO-ELECTRONIC PROPERTIES OF III-V GROUP BINARY SOLIDS

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Received-15.09.2024 **Revised-25.09.2024** **Accepted-30.09.2024** **E-mail : aaryvart2013@gmail.com**

Abstract: The III-V group binary solids, composed of elements from groups III and V of the periodic table, exhibit remarkable optoelectronic properties that have positioned them as foundational materials in advanced semiconductor technologies. These compounds, such as GaAs, InP, and AlN, are characterized by direct bandgaps, high electron mobility, and excellent thermal and mechanical stability, making them ideal for applications in optoelectronic devices, including light-emitting diodes (LEDs), laser diodes, photodetectors, and high-speed transistors. This study explores the fundamental optoelectronic properties of III-V binary solids, focusing on their band structure, optical absorption, carrier dynamics, and response to external stimuli such as temperature and pressure. Computational modeling and experimental data are combined to analyze the impact of lattice structure, alloying, and doping on their electronic and optical behavior. The findings underscore the potential of these materials in the development of next-generation photonic and electronic devices, particularly in communication, energy, and sensing technologies. Additionally, challenges in synthesis, cost, and integration with existing platforms are discussed, along with potential strategies for overcoming these hurdles.

Key words: Optoelectronic properties, GaAs, InP, AlN, semiconductor, photonic & electronic

Introduction: The structural and optical properties of binary semiconductors, including optical, electronic, elastic, and thermal properties, have been the subject of significant experimental and theoretical research in recent decades. Because these semiconductors have the potential to be used in a variety of opto-electronic devices like integral circuits, detectors, lasers, light emitting diodes, modulators, and filters [1-6], the inter-atomic force constant, energy gaps, and consequently the ionicity of III-V group binary solids have been important parameters to study.

When discussing problems in the areas of elastic constants, cohesive energy and heat of formation, bulk-modulus, microhardness, and crystal structures [7-11], crystal ionicity is one of the most significant key parameters of semi-conducting materials. For the case of simple compounds, various theories and calculated ionicities have been developed by Phillips, Van-Vechten, Levine, and a number of other researchers [15-16]. The contributions of the homopolar gap and heteropolar gap to the chemical bond in binary solids have been calculated by Phillips and Van-Vechten. This theory is based on Penn's [17] simple on electron model, which has been used to divide the average energy gap into parts that are homopolar and parts that are heteropolar. It is assumed that the homopolar energy gap is only a function of the distance between nearest neighbors. The Phillips and van-vechten (PVV) theory for ternary chalcopyrite semiconductor compounds has been extended by Levine's [7-11] research to take into account the impact of d-core electrons as well. Levine's bond charge model theory's justification was presented by Singh and Gupta [18]. Both Leven's modification and PVV theory make it abundantly clear that the value of the homopolar energy gap (Eh) is influenced by the distance to the nearest neighbor, whereas the value of the heteropolar energy gap (Ec) is a function of both the distance to the nearest neighbor and the valence electron that is a part of the bond formation. Kumar and others Because it is directly related to the effective number of valence electrons in a compound, 19-21] have calculated the homopolar energy gaps in terms of valence electron plasma energy. Therefore, we believe that the current work should investigate the new modified direction theory of solids proposed by Singh and Gupta [18]. Only the nearest neighbor distance and the number are included in the altered model. for the calculation of III-V group semiconductor compounds' optical properties, valence electrons are required as input.

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Computational Method:

Crystal ionicity and covalency are clearly depicted by several researchers. In the ionic picture, electrons are transferred from one atom to another, resulting in two closed shell ions that interact primarily through Coulomb force and short-range repulsion. In the covalent picture, electrons are shared between atoms rather than transferred. Pauling [22] used the thermo-chemical effect as the primary method for determining the crystal ionicity. A theory based on the one electron model was proposed by Penn [17]. Penn says that the relation given as – can be used to evaluate the average energy gap (Eg= Ep).

$$E_p = \frac{\hbar\omega_p S_0}{\sqrt{\varepsilon_\infty - 1}} \qquad \text{-------(6.1.1)}$$

Here, the relation- provides the valence electron plasmon energy $\hbar\omega_p$.

$$\hbar\omega_p = 28.8\sqrt{\frac{N_{eff}.d}{M}} \qquad \text{-------(6.1.2)}$$

where N_{eff} - is the no. of valence electrons that contribute to the Transformations, ε_∞– the optical dielectric constant and the variable parameter S0 = 0.62.

The average energy gap E_g can be divided into a heteropolar (E_c) and homopolar (E_h) part according to the relation defined by [12-16, 18]-

$$E_P^{\ 2} = E_h^{\ 2} + E_c^{\ 2} \quad \text{(eV)} \qquad \text{-------(6.1.3)}$$

$$\text{and crystal ionicity as } \left(f_i = \frac{E_c^{\ 2}}{E_P^{\ 2}} \right) \qquad \text{-------(6.1.4)}$$

The directly screened potential difference between the fields produced by the ions core of two atoms participating in a given bond at the bond center is represented by the homoploar portion of Eg, which is related to ionic binding [22]. Ec can be obtained from the following relation as, in accordance with modified PVV theory [18]:

$$E_c = \frac{be^2(Z_A - Z_B)}{r_0}\exp(-K_s.r_0) \quad \text{(eV)} \qquad \text{-------(6.1.5)}$$

The nearest neighbor distance r_{AB} is all that matters for the homopolar portion of E_h as

$$E_h = \frac{40.468}{r_{AB}^{\ 2.5}} \quad \text{(eV)} \qquad \text{-------(6.1.6)}$$

K_s is the Thomas-Fermi screening parameter, $r_0 = r_{AB/2}$ is the inter-atomic separation between atoms A and B, rAB is the valence and covelent radii of atoms A and B, and b is an adjustable parameter. For a tetrahedral co-ordination with four bonds, b has a value of 1.5, while for an octahedral co-ordination with six bonds, b has a value of 2.25—1.5 times the ratio of the co-ordination numbers of the two structures, or 6/4. Levine provided an empirical relationship between b and the average co-ordination number N_c^2 (b = 0.089 N_c^2) based on in-depth research into various systems. Therefore, the length of the bond and the number of bonds that emerge from the cation determine the values of E_h and E_c.

We have determined the values of E_h, E_c, and E_p for these materials by applying the equation (6.1.3.- 6.1.6). There are eight electrons per molecule, with three for B, Al, Ga, and In and five for N, P, As, and Sb determining the value of Ks. 1.424 has been chosen as b's value. Table-6.1.1 displays the values that were determined for the aforementioned parameters. The ionicity values determined by Tubb's [23] and other comparable theoretical findings [24-26] are contrasted with the value of ionicity (fi) determined by the Phillips model. The evaluated values were contrasted with those from the Pauling ionicity model and Tubbs' ionicity model, respectively,[23a].

$$f_i = E_p/\hbar\omega_p \qquad \text{(Tubbs)} \qquad \text{-------(6.1.7)}$$

$$f_i = 1 - \frac{1}{6}\exp\{-\frac{(X_A - X_B)^2}{4}\} \qquad \text{(Pauling)} \qquad \text{-------(6.1.8)}$$

where X_A and X_B represent the electro-negativities of atoms A and B. Table 6.1.2 demonstrates that the various ionicities agree very well. However, in comparison to other such theoretical findings, the Phillips ionicity is closer to the Tubb ionicities.

Using the relation (6.1.1) & (6.1.2), the calculated values of plasma energy ($\hbar\omega_p$, in eV) is presented in the Table -6.1.3 along with the values obtained by different researchers [26, 27]. From this table, it is clear that the relation –(6.1.2) is more appropriate to investigate the values of valence electron plasmon energy compared to relation -(6.1.1), because it gives a very good agreement with the reported theoretical findings.

On the basis of Phillips and Van-vechten theory [12-16] and Levine's bond charge model [10, 11], Chemla [28] has described the average bond polarizability for binary compounds having Zinc-Blende (ZB) structure in terms of E_g or E_p, which can be extended to these semiconductor compounds. The polarizabilities (α) for III-V group semiconductors can be computed using the relation as follows -

$$\alpha_{Chemla} = \frac{(2a_0)^3 E_0^2 D_{AB}}{E_g^2} \qquad \text{------(6.1.9)}$$

where α_{Chemla} - is the polarizability of *AB* bonds in III-V group binary solids, m and e are the mass and charge of the electron respectively, $D(AB)$ is the correction factor for *AB* bonds introduced by Van-Vechten [15, 16] to take into account the contribution of the core *d*-electrons. The local field effects are automatically taken into account in Eq.-(6.1.9) by assuming the value of energy gap determined by Phillips and Van-Vechten [12-16].

In the present model, the energy gap of the bonds, E_p, has been calculated using the relations, recently developed by the authors [12-16] between the homopolar energy gap and heteropolar energy gap in term of inter-atomic separation for III-V group binary solids.

The well-known phenomenological method of the Classius and Mossotti relation has also been used to calculate the electronic polarizabilities. As a result-

$$\alpha_{CM} = 0.395 \times \frac{(n^2 - 1)M}{(n^2 + 2)d} \times 10^{-30} \qquad \text{---------(6.1.10)}$$

where M-molecular weight, d-density, and ($n = \sqrt{\varepsilon_\infty}$) are the materials' estimated refractive indexes from relation –(6.1.1), which are listed in Table 6.1.4 and an optical dielectric constant (ε_∞) are listed in Table 6.1.6, respectively. The computed values of electronic polarizability using Chemla's relation and Claussius-Mossotti relation are presented in the Table-6.1.5 along with the values investigated by different investigators [30, 31]. The values of the polarizability that were calculated using eqns are fairly consistent, as shown in Table 6.1.5. 6.1.9) and 6.1.10) for the binary compound semiconductors of the III-V group.

Using the aforementioned relations, E_h, E_c, and E_g, the ionicity (f_i) of binary compound semiconductors from the III-V group is evaluated. The micro-hardness (H- in GPa), which is given by the following relation proposed by Neumann's [32] for binary semiconductors with tetrahedral co-ordination, was evaluated using the computed values of various ionicities produced by the Phillips and Tubb's model: -

$$H = h_0 T_m a^{-2.633} (1 - g_0 f_i) \qquad \text{------(6.1.11)}$$

Where "the adjustable parameter h_0 have different values for different type of semiconductors compounds and for the III-V group binary compound semiconductors has values $h_0 = 0.62$ & $g_0 =$

1.283, *a*- lattice constant and T_m – melting temperature these III-V group binary compounds"[29]. The computed values of micro-hardness using above relation are presented in the Table- 6.1.7 and compared with the reported theoretical and experimental data [33, 34, 35]. The agreement is very good between the various ionicities and hence with the reported theoretical and experimental values.

COHESIVE ENERGY: The cohesive energy gained in the solid's ground state in relation to its component a neutral free atoms can be determined by utilizing the derived values of various ionicities of these semiconductor compounds. As a result, [78] can be written-

$$U = \frac{\log_{10}(1-f_i)}{K} \times T_m \qquad \text{------(6.3.12)}$$

where K can be changed and can have different values for $A^N B^{8-N}$ (N=1, 2, 3) semiconductor binary compounds. The various ionicities derived from Phillips and Tubb's ionicity model are represented by the variable K for these semiconductor compounds 1.4×10^2 and f_i — is the parameter. Table-6.1.8 contains the results of this relation, which are found to be more consistent with experimental data [37] and other theoretical findings of this kind [33, 38].

BULK MUDULUS: The Scaling relation of Neumman provides the bulk modulus [39].-

$$B = B_0 V^{-n} \qquad \text{-------(6.1.13)}$$

where n is 1.147, the factor B0 is as follows: $B_0 = b_0\ (1\text{-}b_1\ f_c)$, where b_0 and b_1 are the adjustable parameters with values of 4.143 and 2.655, respectively, and fc is the covalency, i.e. fc = $[1\text{-}(E_c^2/E_g^2\ )]$. The computed values of bulk-modulus from various ionicities are presented in Table-6.1.9 and are also compared to the experimental data [37] and other such theoretical findings [33, 38].

Using the investigated values of various ionicities, lattice energy of these materials are computed by the following relation as-

$$U_{lattice} = 1447.6 – 370.5\ (\hbar\omega_p)^{-0.667} \qquad \text{-------(6.1.14)}$$

The detailed theory of this expression discussed in the ctaptor-3. the computed values of this parameter is presented in the Table-6.1.10 along with the reported values [A, B, C, D]. For these binary compound semiconductors, the values reported in this table and the values calculated from the lattice energy using relation (6.1.14) agree fairly well, as can be seen from this table. Using the investigated values of average energy gap and plasmon energy from the relations (6.1.2) & (6.1.3), the optical susceptibility of these materials is to be determines by the relation [8]-

$$\chi_o = 7.96 \times 10^{-2}\ (\hbar\omega_p/E_g)^2 \qquad \text{-------(6.1.15)}$$

The computed values of these semiconductors are presented in the table- 6.1.11 along with the theoretical values [37] and experimental values [40]. The agreement is fairly good between them.

RESULTS AND DISCUSSION: The values of the investigated Penn gap (E_p), homopolar gap (E_h), and heteropolar gap (E_c) for III-V group binary compound semiconductors are listed in Table-6.1.1 on the basis of the present investigation. Using Phillips' ionicity model, the values of ionicity (f_i) for Boron, Aluminum, Gallium, and Indium pinictides were calculated and compared to those of Tubbs' and Pauling's ionicity models, as well as those of other researchers. The calculated numerical results of these materials' ionicities are shown to be in good agreement with the values obtained from Phillips and Tubb's model and thus with other such theoretical findings [18, 45, 62] in Table-6.1.2. Thus, it may seem that the Phillips ionicties is more appropriate to than ionicity values from Pauling's model. The computed values of plasmon energy ($\hbar\omega_p$) using eqn.-(6.1.2) are shown in Table-6.1.3 along with the values reported by [****] and the agreement is found very good between them. From equations, the values of electronic polarizability AB were calculated. 6.1.9) and (6.1.10) are also shown in Table 6.1.6, and we also find that there is a fairly good agreement here. We compare the calculated values of micro-hardness H (in GPa) to those that have been reported in the literature in Table 6.1.7. The cohesive energy U and bulk modulus B calculated with various ionicities (f_i) are shown in Table 6.1.8 and 6.1.9, respectively, along with the theoretical and experimental values that have been reported [33, 38]. H (measured in GPa), U (measured in Ryd. per electron) and B (in 10^{-12} dyne-cm^{-2}) that were calculated from the various ionicities (Phillips and Tubbs) are closer to the experimental data than the values that were derived from various researchers. The calculated values oflattice energy ($U_{lattice}$), optical susceptibility (χ_0) and magnetic susceptibility (χ_0) are investigated using the relations (6.1.14 to 6.1.16) and are presented in the table- 6.1.10, 6.1.11 & 6.1.12 respectively. The available theoretical and experimental data of these parameters are also given in their respective table. As a result, we believe that, in comparison to other theoretical findings, the values of various ionicities derived from the Phillips and Tubbs models are more appropriate.

CONCLUDING REMARKS: For III-V group binary compound semiconductors, the values of E_h, E_c, and E_p have been investigated using the Phillips and Van-Vatchen theory. It has been demonstrated that the values derived from the Penn model and the Phillips model are in agreement with the values found in the investigation. Electronic polarizability and Phillips ionicity have been derived from the calculated data for further verification. The values derived from the Clausius-Mossotti relation were also found to be very consistent with the derived polarizability. We were able to determine the bulk modulus (B), cohesive energy (U), and microhardness (H) of these materials using the Phillips ionicity values, which were found to be in good agreement with the reported experimental data and the values reported by various researchers. The lattice energy, optical susceptibility, and magnetic susceptibility of these materials are also determined by the plasma energy and average energy, which are very important parameters. In light of the foregoing, we conclude that the theory of Phillips and Van-Vechten holds true for zinc-blende structures in III-V group binary tetrahedral semiconductors.

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