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Research Article

Adjusted Adashi's Model of Exciton Bohr Parameter and New Proposed Models for Optical Properties of III-V Semiconductors

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Abstract

The energy gap of the semiconductor changes dramatically with its size. Consequently the determination of the correlation between the exciton Bohr parameter (a_B), which is a size parameter, and the energy gap (E_g) is a main property for understanding the behaviour of the nanostructure properties. In this work, we propose the adjustment of Adashi's model of exciton Bohr parameter with energy band gap to III-V family of semiconductors and propose new numerical models linking the exciton Bohr parameter (a_B) to the optical properties such as the refractive index (n) and the dielectric constant (ε). We found that our predictions will be more accurate for this family of semiconductors. Our objective is to propose some models which corresponding to bulk semiconductors and giving predictions to semiconductor nanostructures.

Keywords: Exciton Bohr parameter; Energy band gap; Refractive index; Dielectric constant

1. Introduction

Semiconductor nanostructures are attracting a great deal of interest as the most promising devices for many nano-technological optoelectronic applications such as quantum information processing, quantum computing and solar cells. In this nanoscale, their electronic and optical properties depend strongly on their size and shape, i.e. on their geometry. Most spectral studies of semiconductor nanoparticles were focused primarily on the lowest excitonic transitions where one can comfortably neglect the presence of strong dispersions in the dielectric response (Krauss and Wise, 1997; Olkhovets et al, 1998; Wise, 2000; Hyun et al., 2010). Following this think, Adachi (2005) proposed a model which gives good prediction for some semiconductors of III-V and II-VI families linking the direct-exciton Bohr parameter (a_B) to the energy gap (E_g) (lowest direct band-gap energy) because exact calculation of the exciton effect at the indirect band gap is quite

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complicated, and it is convenient at this stage to make approximations and consider a more specific model (Adachi, 2005). It has also been the subject of other previous studies. Therefore to our knowledge, the correlation of the size through the exciton Bohr parameter to the optical properties for specific family of semiconductors has not been done yet.

Our purpose, in the first step, is to calculate the electronic band gaps of all III-V binary compounds using a standard semi-empirical sp^3s^* tight binding method and to adjust Adashi's model for III-V family of semiconductors which involve these lowest band gap energies (E_g). In the second step we propose new numerical models specific to III-V semiconductors linking the exciton Bohr parameter (a_B) to the optical properties such as the refractive index (n) and the dielectric constant (ε). Because the Coulomb interaction is always present between electrons and holes, excitonic transitions play an important role in the fundamental optical process of semiconductors (Elliott, 1957).

2. Calculations and results

2.1 Electronic band structures

We first provide a method to determine the band structure of binary III-V semiconductors with emphasis placed on accurate determination of the principal energy gaps (Roessler and Swets, 1978). This method includes only five basic orbitals (s, s^*, p_x, p_y, p_z) per atom, the usual sp^3 basis plus one excited s^* orbital. The inclusion of this excited state is physically important for reproducing accurate indirect gap edges. For each wave vector k in the Brillouin zone, the Bloch function can be constructed by a linear combination of atomic orbitals.

$$|n_b k\rangle = N^{-1/2} \sum_{i,b} exp[ik(R_i + \tau_b)]|\, n_b R_i\rangle \qquad (1)$$

Where n is a quantum number that runs over the basis orbitals s, s^*, p_x, p_y and p_z on the different types of site b in a unit cell (we shall consider the two sites a and c in the unit cell as anion and cation sites, respectively). The N of wave vector k lies in the Brillouin zone. R_i represents the position of the atom in the unit cell. The electronic eigenstates of the zinc blend structure are expended as:

$$\sum_{m,b'}\left[\langle n_b k|H|n_{b'},k\rangle - E(k\lambda)\delta_{n,m}\delta_{b,b'}\right]\langle m_{b'},k|k\lambda\rangle = 0 \qquad (2)$$

λ denotes the band index, and $E(k\lambda$ is the eigenwave functions which can be obtained by solving the Schrodinger equation:

$$\big(H - E(k\lambda)\big)\big|k\lambda\rangle = 0 \qquad (3)$$

In this paper only the nearest-neighbor interactions are included. We model the band structure of the binary semiconductors using the Vogl et al. (1983) sp^3s^* tight-binding parameters. The determination of matrix element values for tetrahedral semiconductors is to determine the band structures at special points and has been described elsewhere. Table 1 exhibits the principal calculated and experimental energy gaps of several III-V binary compounds; there is a good agreement with the theoretical data. GaAs and GaSb are direct gap semiconductors, GaP is indirect

gap, InAs resembles in its band structure InSb (direct gap), InP is a direct gap semiconductor, and InN is a direct gap at Γ, closely similar to that of GaN. AlAs is an indirect wide gap semiconductor with a band structure similar to those of AlP and AlSb. BAs, BN and BP are an indirect gap.

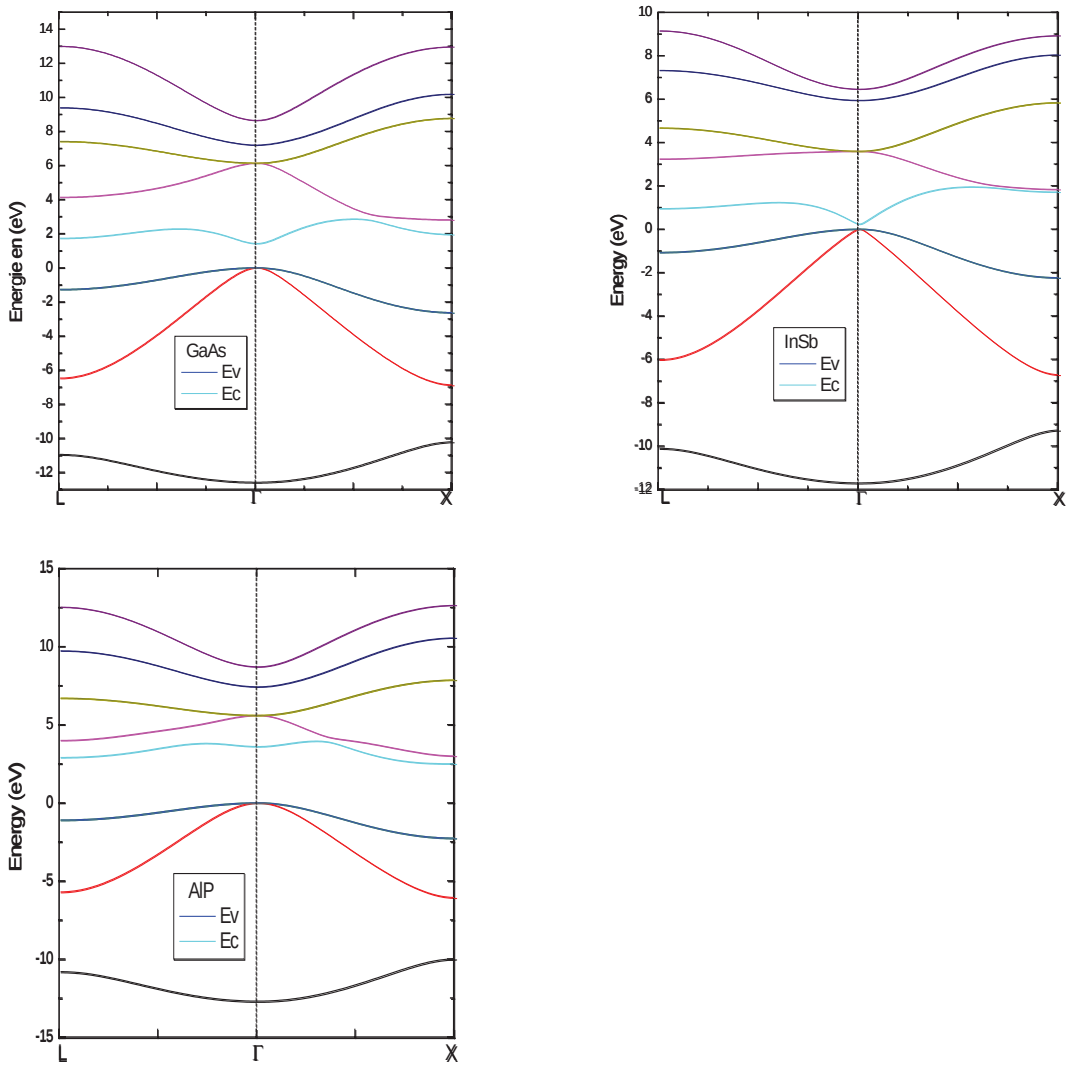


Fig 1. Band structures of III-V binary compounds Ga-V (GaAs), In-V (InSb) and Al-V (AlP)

Table 1 Our calculated direct (D) and indirect (ID) band gaps (eV) of the III-V binary semiconductors at T=0 and 300 K, and compared with experimental data at T=300 K.

Compounds	Nature	Eg_{min} calc.		Eg_{min} exp
		0 K	300 K	
GaAs	D	1.519	1.419	1.42[a]
GaSb	D	0.813	0.725	0.72[a]
GaP	ID	2.35	2.272	2.26[a]
β-GaN	D	3.28	2.203	3.17[b]
InAs	D	0.429	0.35	0.43[c]
InSb	D	0.243	0.17	0.23[d]
InP	D	1.423	1.34	1.423[c]
InN	D	0.77	0.77	0.77[d]
AlAs	ID	2.299	2.153	2.30[e]
AlSb	ID	1.61	1.615	1.609[e]
AlP	ID	2.5	2.45	2.5[c]
c-AlN	D	6.19	6.2	6.13[d]
BAs	ID	0.67	0.67	-
BSb	D	0.527	0.527	-
BP	ID	2.11	2.1	-
c-BN	ID	6.345	6.345	6.2[c]

a: (Rabah et al., 2003), b: (Velasco et al., 2003), c: (Vogl et al., 1983), d: (Adashi, 2005), e: (Rabah et al., 2001)

2.2 Adjusted Adashi's model for band gap

The Bohr exciton radius of such bound electron-hole pair is defined as:

$$a_B = \frac{\hbar^2 \varepsilon_0 \varepsilon_s}{\mu e^2} (\mathring{A}) \qquad (4)$$

This a_B symbolizes the characteristic length scale to observe quantum effects in nonmaterial.

In obtaining equation (4), we assumed that the relative dielectric constant is equal to the static dielectric constant ε_s. This is because the exciton binding energy is usually smaller than the lattice vibrational (LO phonon) energy in many semiconductors. If not so, we must use ε_∞ instead of ε_s, where e is the electronic charge, $\hbar$ is the reduced Plank's constant, $\mu = \left(\frac{m_e^* m_h^*}{m_e^* + m_h^*}\right)$ is the reduced mass of electron-hole bound state, m_e^* and m_h^* are effective mass of electron and holes respectively in M.K.S.A. units.

Where $a_B^{HD} = \frac{\hbar^2 \varepsilon_0}{m_0 e^2}$ is hydrogenic Bohr radius, the free-electron mass m_0 replaced by the exciton reduced mass μ. So:

$$a_B = a_B^{HD} \frac{\varepsilon_s}{\mu / m_0} (\mathring{A}) \quad (5)$$

It should be noted that the indirect exciton Bohr radius can be expressed by the same expression as equation (5).

Using Eq. (5) for direct and indirect exciton Bohr radius, we have calculated the 1st-orbital (n = 1) Bohr radius a_B for III-V semiconductors. We have plotted in Fig. 2 the variation of this quantity as a function of the energy band gap E_0 (lowest band-gap energy) at T=300K in order to give a good connection between them. We can see that the a_B decreases with increasing E_0. Our obtained results correspond to the following relation:

$$a_B = \left(\frac{A}{E_0} \right)^{\alpha} \quad (6)$$

Where $A = 44.594\ eV$ and $\alpha = 1.288$ are our parameters specific to III-V semiconductors.

This relation is then our adjustment of Adashi's model specific to III-V semiconductors. This is can be seen clearly in the Fig. 2 when the comparison is made with the Adashi's model, the calculated exciton Bohr parameter from equation 5 and the experimental data. We must notice here that the Adashi's model is universal to III-V and II-VI semiconductors, and also follows the same relation given by Eq (6), but with parameters $A = 66.9\ eV$ and $\alpha = 1.18$. We have illustrated in Fig. 3 this comparison from the relative error obtained for our results and Adashi's model. The error is significantly smaller with our results for the most studied compounds. This shows that our adjustment is more closed to the experimental data compared to the Adashi's model. This obtained improvement is valuable only for III-V semiconductors and does not guarantee for other families of semiconductors because of the high variation of the ionicity and the band gap observed in them (going from IV to II-VI groups).

In Table 2, we list our calculated 1st-orbital (n = 1) Bohr radius a_B obtained from our adjusted results and using Eq. 5, compared Adashi's model and experimental data for III–V semiconductors. It is well shown the good improvement of our adjustment. The BSb and InN have values which are not well comparable to the models and are far from the slope of the Fig. 2. For this reason we have neglected them in order to decrease the errors in the adjustment.

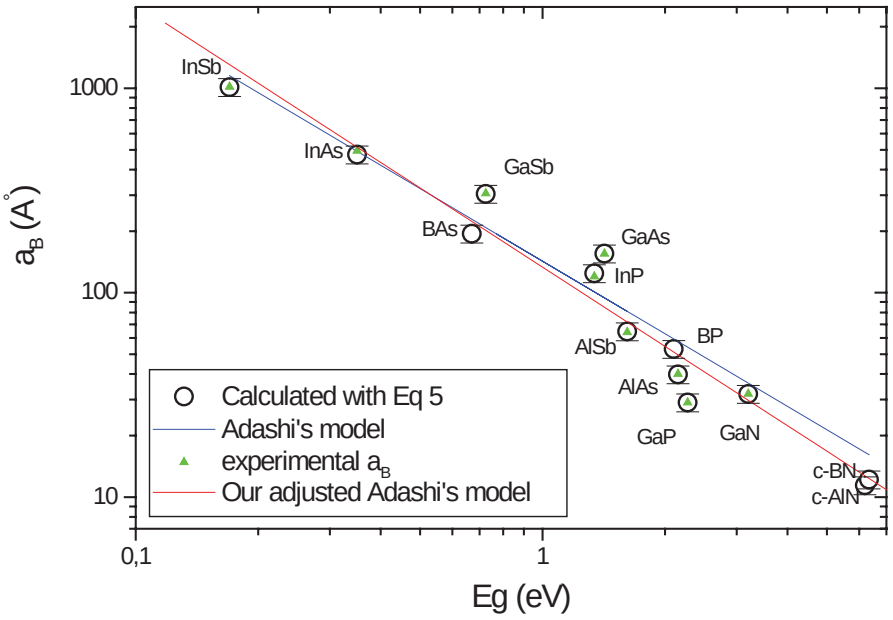


Fig 2. Exciton Bohr radius a_B versus energy E_g for III–V semiconductors at T=300K.

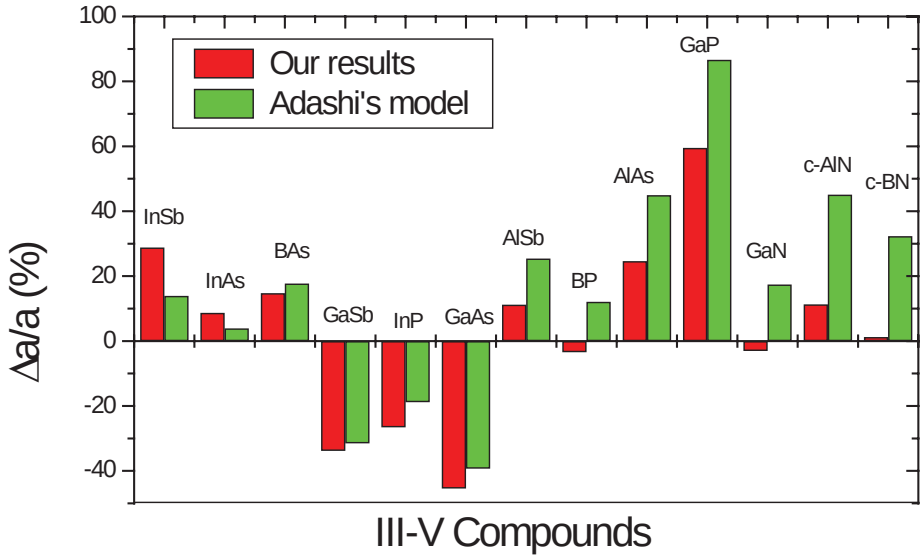


Fig 3. Comparison of the relative error of the exciton Bohr parameter with our adjusted results and Adashi's model for III-V semiconductors.

Table 2 Exciton Bohr parameter a_B (in Å) for some III–V semiconductors at T=300K:

Compounds	a_B			
	(Our adjustment)	(Adachi's model)	(Calculated Eq. 5)	(Expt.(Adashi,2005))
GaAs	84.823	94.332	155.386	155
GaSb	201.443	208.355	304.259	306
GaP	46.261(ID)	54.130	29.005	29 (ID)
	35.672(D)	42.66	50.258	50(D)
β-GaN	29.724	36,094	31.935	32
InAs	514.645	492.042	473.687	494
InSb	304.517	1153.647	1012.888	1017
InP	91.318	100.929	124.309	120
InN	186.409	194.063	78.728	-
AlAs	49.580(ID)	57.678	39.789	40 (ID)
	30.494(D)	36.950	55.000	55 (D)
AlSb	71.802(ID)	80.976	64.579	64(ID)
	47.628(D)	55.600	457.00	445(D)
AlP	41.978	49.520	-	-
c-AlN	12.696	16,556	11.141	-
BAs	222.989	228.683	194.333	-
BSb	303.791	303,575	52.337	-
BP	51.197	59.399	53.000	-
c-BN	12.323	16.111	12.175	-

2.2 New models for optic properties

The refractive index n is a very important physical parameter related to the microscopic atomic interactions.

We have used the Moss et al model (Hervé and Vandamme, 1994) based on the atomic model, which relates the refractive index n to the energy band gap E_0 of the semiconductors, as follows:

$$n^4 E_0 = k \qquad (7)$$

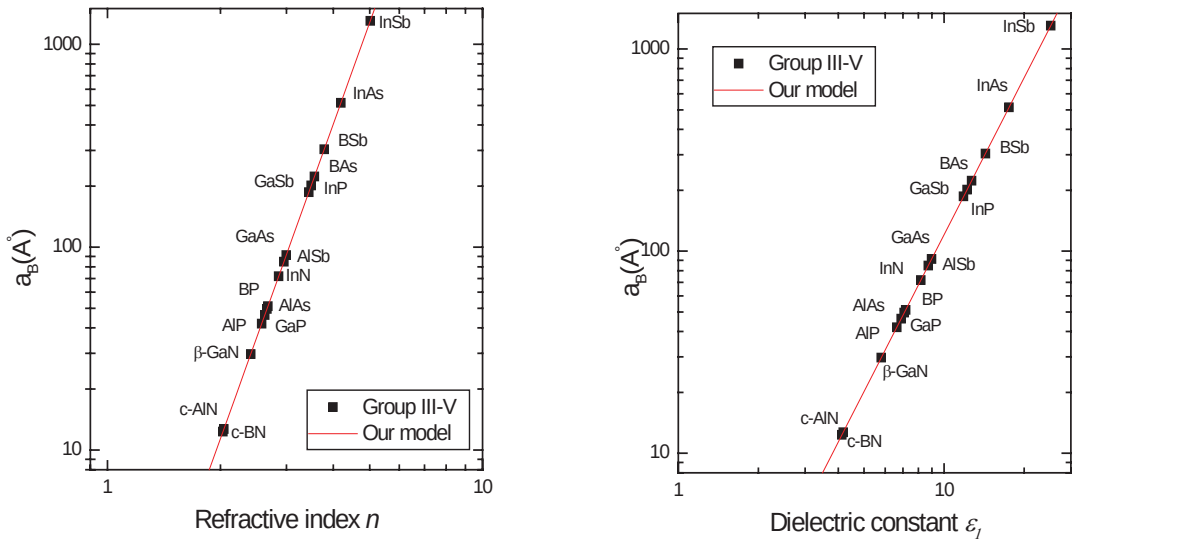
Where the constant k= 108 eV is determined by Ravindra and Srivastava (1979). If the absorption of the medium is weak, we can deduce the real dielectric constant as $\varepsilon_1 = n^2$. To our knowledge, no information is published showing how the exciton Bohr radius behaves as function of the optical properties. Therefore, we have aimed to predict the relations between the exciton Bohr radius and the refractive index and the dielectric constant for III-V semiconductors. As displayed in Fig. 4 (a,b), a direct increase behavior is observed. Our results for the refractive index correspond, finally, to the following relation:

$$a_B = \left(\frac{n}{B}\right)^{\beta} \tag{8}$$

where $B = 5.242$ and $\beta = 5.152$ are our obtained parameters. And for the dielectric constant, the corresponding relation for our results is given by:

$$a_B = \left(\frac{\varepsilon_1}{C}\right)^{\delta} \tag{9}$$

where $C = 1.556$ and $\delta = 2.576$ are our obtained parameters.



a) **b)**

Fig 4. (a) Exciton Bohr radius a_B versus refractive index n for III–V semiconductors; (b) Exciton Bohr radius a_B versus dielectric constant ε_1 for III–V semiconductors.

3. Conclusion

We have proposed an adjustment of Adashi's model of the exciton Bohr parameter a_B as function of the band gap E_g, to be specific to the III-V family of semiconductors. New numerical models linking the exciton Bohr parameter to the optic properties such as the refractive index n and the dielectric constant ε_1 are then proposed. For the energy band gap, we have found that our adjustment is more accurate for this family of semiconductors than the Adashi's model developed for III-V and II-VI families, compared with experimental data and calculated ones. For the refractive index and the dielectric constant, our proposed models are predictions since to our knowledge, no information are published about this subject. Our proposed models correspond to bulk semiconductors and give predictions to semiconductors nanostructures through the dependence with the size.

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