

# Electronic Properties of $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$ Quaternary Semiconducting Alloys Lattice Matched to GaAs

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Based on a pseudopotential approach under the virtual crystal approximation, the electronic properties, namely the electronic band structure, direct and indirect energy band gaps, valence band width, and antisymmetric band gap of  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$ , lattice, matched to GaAs, have been investigated. A detailed comparison is made between our results and previously reported data, wherever possible. In other cases our results are predictions. Our findings show that by varying  $x$  and/or  $y$ , diverse values can be obtained for the electronic parameters of interest.

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## 1. Introduction

Semiconducting alloys give the possibility to choose material properties by selecting appropriate alloy constituents [1–5]. This could lead to new semiconducting materials with energy band gaps covering a continuous broad spectrum. In ternary semiconductor alloys, the lattice parameter and energy band gap change with each other [6–11]. However, several applications need the choice of these both parameters independently. This shortcoming can be overcome by using quaternary semiconductor alloys. The use of III–V quaternaries have opened up new generations of device applications [12–18]. On the other hand, alloying with the group III-nitrides are of particular importance [19–22]. This is due to the large difference between the energy band gaps of the quaternary alloy constituents.

$\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$  belong to III-nitride quaternaries. These alloys are formed from AlN, AlAs, GaN, and GaAs binaries and can be grown lattice matched to GaAs substrate. These have found numerous applications in optoelectronic devices [23–27]. The electronic band structure is an effective means for describing the electronic properties of semiconductor materials [28–30] and an accurate determination of band parameters of a material permits a precious knowledge for its synthesis and devices fabrication [1, 14]. The present contribution deals with the electronic properties of  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$  quaternary semiconductor alloys lattice method to GaAs. The aim of this work is to obtain material properties that differ strongly from those of conventional III–V alloys by varying  $x$  and  $y$  concentrations.

## 2. Computational method

The calculations are performed using the empirical pseudopotential method (EPM) [28, 29, 31] under the virtual crystal approximation (VCA). In the EPM, a set of atomic form factors are treated as adjustable parameters, which are fitted to available experimental data in the literature. The experimental energy band gaps used in the fitting procedure for AlAs, AlN, GaN, and GaAs are given in Table I [15, 32–34]. Numerical calculations are done along the principal directions of symmetry of the Brillouin zone. Our eigenvalue problem has a dimension of  $136 \times 136$  matrix. The pseudopotential form factors (PPFFs) are optimized using the non-linear least-squares method, as described in Refs. [35–37]. The final adjusted PPFFs along with used lattice parameters for binary compounds of interest are listed in Table II.

The lattice parameter of quaternaries is assumed to follow Vegard's law [38]. The lattice matching condition for  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$  on GaAs substrate is

$$y = \frac{0.01x}{1.15 + 0.14x}, \quad 0 \leq x \leq 1 \quad \text{and} \quad 0 \leq y \leq 0.0078. \quad (1)$$

TABLE I

Experimental band-gap energies fixed in the fits for AlN, AlAs, GaN, and GaAs.

Compound	$E_{\Gamma-\Gamma}$ [eV]	$E_{\Gamma-X}$ [eV]	$E_{\Gamma-L}$ [eV]
AlN [32]	6.0	4.9	9.3
AlAs [15]	2.95	2.16	2.36
GaN [33]	3.3	4.5	6.0
GaAs [34]	1.42	1.91	1.73

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Pseudopotential parameters for AlN, AlAs, GaN, and GaAs.  $V_S$  denotes the symmetric pseudopotential form factors, whereas  $V_A$  denotes antisymmetric pseudopotential form factors.

Compound	Form factors [Ry]						Lattice constant $a$ [Å]
	$V_S(3)$	$V_S(8)$	$V_S(11)$	$V_A(3)$	$V_A(4)$	$V_A(11)$	
AlN	-0.309603	0.112783	0.067538	0.28	0.33	0.015	4.37
AlAs	-0.212694	0.00	0.092750	0.068833	0.05	-0.0075	5.6611
GaN	-0.347240	-0.016	0.21217	0.159988	0.200	0.135	4.50
GaAs	-0.239833	0.0126	0.059625	0.060536	0.05	0.01	5.6533

### 3. Results and discussion

In Fig. 1, we plot the electronic band structure of zinc-blende  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$  lattice matched to GaAs with  $x = 0.1$ . The energy zero is taken to be at the top of the valence band. Note that both the valence band maximum and the conduction band minimum are located at the  $\Gamma$  point, thus indicating that the material of interest is a direct band-gap semiconductor. The general features of this band seem to be similar to those of III-V semiconductors [28, 39, 40]. The main difference lies in the magnitude of the fundamental band gap.

The variations of the direct  $\Gamma$ - $\Gamma$ , coming from the top valence band state and lowest conduction one at the Brillouin zone center, and indirect  $\Gamma$ - $X$  and  $\Gamma$ - $L$ ) energy band gaps which are identified as the energies of the lowest conduction states at  $k = 2\pi/a$  (0.5,0.5,0.5) and  $k = 2\pi/a$  (1,0,0), respectively ( $a$  is the lattice constant), are measured from the top of the valence band at zone center. They are displayed in Fig. 2 as a function of aluminum concentration  $x$  for  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$ . We observe that when  $x$  increases from 0 to 1, all band gaps of interest increase as well. The quadratic least-squares fits to our data have given optical bowing parameters for the band gaps at  $\Gamma$ ,  $X$ , and  $L$  of  $-0.12$ ,  $-0.19$ , and  $-0.154$  eV, respectively. These parameters are induced by composition disorder. The extent of the direct-to-indirect-band-gap transition has been examined. Our results showed that a transition from a direct to indirect gap occurs at  $x \approx 0.34$ . This transition is originated by  $X$ -conduction band.

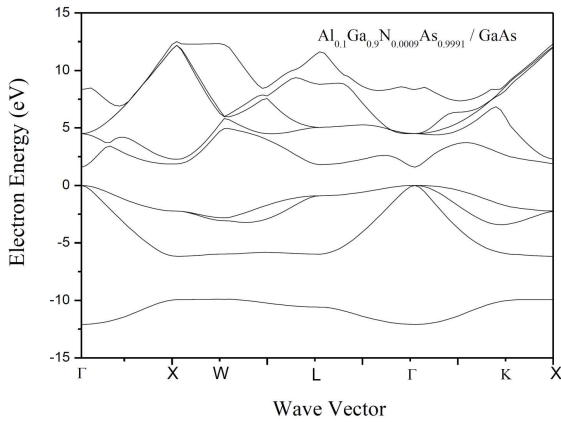


Fig. 1. Electronic band structure of  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$  with  $x = 0.1$ .

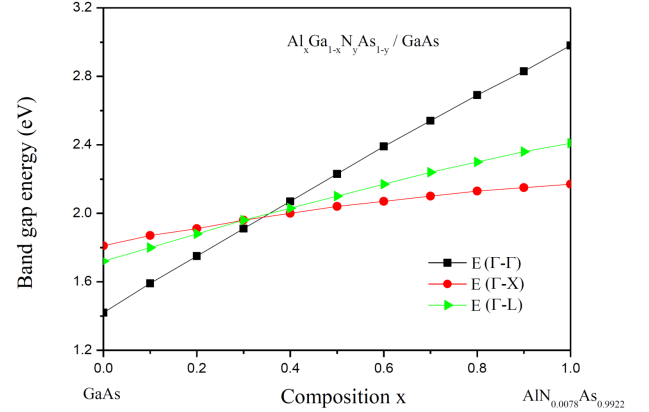


Fig. 2. Direct and indirect band-gap energies in  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$  versus  $x$ .

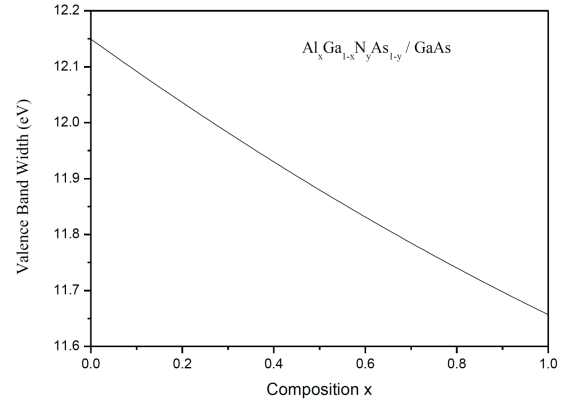


Fig. 3. Valence band width in  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$  versus  $x$ .

Figure 3 illustrates the variation of the valence band-width (VBW) for  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$  versus the aluminum content  $x$ . We notice that VBW decreases with increasing  $x$  from 0 to 1. Hence, the addition of more aluminum atoms in a  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$  causes narrowness in the VBW. This could be attributed to the interaction between the  $s$  and  $p$  electrons of nitrogen with  $d$  electrons of the system and the change in the valence electrons' binding energy.

One of the important parameters that can make a general distribution between covalent and ionic bonding in semiconducting materials is the ionicity [41, 42]. The

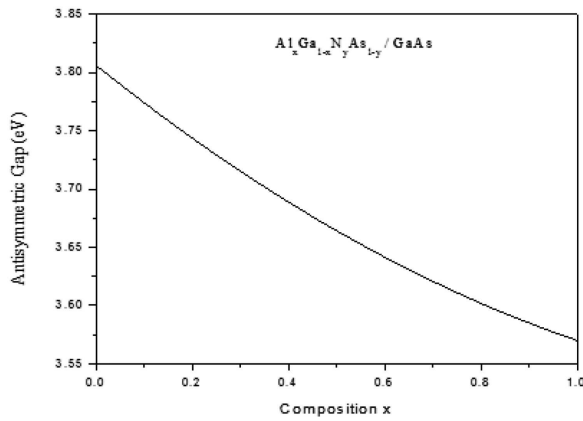


Fig. 4. Antisymmetric gap in  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$  versus  $x$ .

gap between the first and second valence bands at  $X$  (see Fig. 1), termed as the antisymmetric gap, has been linked to the ionicity in such a way that the increase (or decrease) of this gap implies the increase (or decrease) of the ionicity [43, 44]. In this respect, the variation of the antisymmetric gap as a function of  $x$  for  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$  is shown in Fig. 4. Note that as  $x$  increases from 0 to 1, the antisymmetric gap decreases. This suggests that by incorporating more Al atoms into  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$  its ionicity decreases (the material becomes more covalent).

#### 4. Conclusion

A pseudopotential study of electronic properties of  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$  quaternaries lattice matched to GaAs substrate for various Al contents  $x$  ( $0 \leq x \leq 1$ ) was reported. Our findings showed that the incorporation of the aluminum into  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$  affects significantly the electronic properties of the material system in question, thus providing more diverse opportunities to obtain desired electronic properties for new electronic devices.

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