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Bond length Distortion in III - V Semiconductors

Kalyan Singh[1], P. K. Sharma[2]

IIMT College of Engineering Greater Noida

[1, 2]Department of Electronics & Communication Engineering, IGDTUW Delhi, India
E-mail: *drpk.sharma21[at]gmail.com*
E-mail: *pankajsharma_gn[at]iimtindia.net*

Abstract: ***Semiconductors are present in periodic table of Group III - V. In this paper, impurities doped with Al- series and Ga-Series such as AlP, AlAs, AlSb and GaP, GaAs, GaSb. The value of distorted bond length found corresponds with orbital parameter, covalance and empirical parameter ang hybrid energy used as input data.***

Keywords: semiconductors, bond length, impurity atom and host atom

1. Introduction

We have investigated bonding properties such bond length distortion of atomic substitution in Al series and Ga – series of III – V group of semiconductors using bond orbital parameters based on tight binding theory with universal parameter. We have studied schematic behavior of lattice distortion with respect to some of the chemical parameters such as co valence difference and electro negativity difference between the impurity atom and host atom and the change in covalent energy of the bond when the impurity replaces the host has been attempted.

Theory: The op to-electronic properties of III – V group semiconductors compounds, V K Singh et., [1-3]. The ideas of simple force constant model suggested by Kraut and Harrison [4-7] have also described a method to estimate the local relaxation is used impurities in semiconductors using just the natural bond length. In this model the second neighbor relaxation of the nearest neighbors. Thus the bond length distortion Δd due to the size difference between the impurity and host atoms in any defect system is given as three fourths difference of the natural bond length of impurity - host and host - host bond.

$$\Delta d = \frac{3}{4}(d_{\text{impurity - host}} - d_{\text{host - host}}) \quad \text{.....(1)}$$

The positive distortion $+\Delta d$ corresponds to the nearest neighbours relaxing outwards and negative distortion - Δd corresponds to the nearest relaxing inwards.

To study bond length distortion of atomic substitutions in semiconductors we have taken Al - series and Ga-series from III - V group of semiconductors. In every compound semiconducting system the cationic substitutions of group II and group III impurities is followed by anionic substitutions of groups V and VI impurities. We studied dependence of the sign extent of bond length distortion of various impurities in different host system.

1) Change in covalent energy of the host - impurity bond with respect to that of host - host bond. The covalent energy V2, which is the potential parameters related with the bond length by the following equation

$$d^2 = \left(\frac{24.532}{V2}\right) \quad \text{.....(2)}$$

The polar energy V3, is related with the bond length by following equation.

$$d = \frac{8.163}{K^2 \in h^2 - 4V^2_3} \quad (3)$$

Where K is an empirical parameters and $\overline{\in_h}$ is the cation - anion average hybrid energy.

2) The difference in electro negativity (ΔT) between the host and that of the impurity atom.

3) The change in covalency ($\Delta\alpha_c$) of the bond when the impurity replaces the host. The covalent energy V2 of the host - impurity bond for Al series and Ga- series of III - V group of semiconductors are reported in table 3 and the rest input data for host compounds are taken from table -4. We have used the values of dhost - host, calculated by us in table 2.

Table 1
The value of bond orbital parameters (V2), Covalence αc, empirical parameter (K) and cation and anion average hybrid energy input data.

$\overline{\in_h}$ (eV)

Table 2

Compound	V2 (eV)	V3 (eV)	αc	K	$\overline{\in_h}$ (eV)
AlP	- 4.465	2.17	0.88	1.45	8.89
AlAs	-4.205	2.04	0.90	1.39	8.75
AlSb	-3.610	1.48	0.84	1.28	8.02
GaP	-4.355	2.00	0.85	1.39	9.02
GaAs	-4.100	1.87	0.87	1.33	8.85
GaSb	-3.535	1.30	0.90	1.22	8.15

Table 3
The values of bond length III - V group of semiconductors

Compound	Present Work		Experimental Values
	Equation - 2	Equation - 3	
AlP	2.34	2.34	2.367
AlAs	2.42	2.42	2.442
AlSb	2.61	2.61	2.657
GaP	2.37	2.37	2.358
GaAs	2.45	2.44	2.448
GaSb	2.63	2.64	2.639

Bond length distortion of impurities in III - V group of semiconducting compound. (Table enclosed)

I. AlP
II. AlAs
III. AlSb
IV. GaP
V. GaAs
VI. GaSb

2. Result and Discussion

We have also studied the bond length distort of atomic substitutions in III - V group of semiconductors. For this purpose we have Al series and Ga - series from III - V group of semiconductors. In every compound semiconducting system the cat-ionic substitutions of group II and III impurities is followed by the anionic substitution of group V and VI impurities. We have studied the dependence of the sign and extent of bond length distortion of various impurities in different host system. We have calculated and reported the values of bond length (impurity host system), bond length distortion and the ratio of bond length distortion to the host bond length. The difference in covalency between host - host bond and host - impurity bond, the ratio of bond length distortion to the covalency difference and the difference in electro-negativity are also calculated and reported in table 3. It is found that the dependence of bond length distortion on bond orbital parameter V2 is same, as on the hybrid energy [8, 9]. The sense of distortion is decided by the sign of the difference in electronegativity between the host and the impurity atom, Viz, an impurity with a higher electro - negativity than the host atom it is replacing, results in a contraction and vice - versa. This is an agreement with the suggestion made by Scheffler et., al. {11 - 12]. It is also suggested that when an impurity enter a semiconductor substitutionally, the resulting bond length distortion is a function of above parameters and not just decided by the difference in size between the impurity and host atoms.

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