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Bond Length and Bond Length Distortion in Zn-Series of II-VI group of Semiconductors

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Abstract: ***Semiconductors are present periodic table of group II-VI, in this paper, impurities doped with Be-series, Zn-series and Cd-series such as BeS, BeSe, BeTe, ZnS, ZnSe, ZnTe and CdS, CdSe, CdTe. The value of distorted bond length found corresponds with orbital parameter, covalence, empirical parameter and hybrid energy used as input data.***
Keywords: Semiconductors, bond length, impurity atom and host atom.

I. INTRODUCTION

We have investigated bonding properties such as bond length distortion of atomic substitution in Be-series, Zn-series and Cd-series of II-VI group of semiconductors. Using bond orbital parameters based on tight binding theory with universal parameters. We have studied schematic behaviour of lattice distortion with respect to some of chemical parameters such as covalency 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.

II. THEORY

The optoelectronic properties of II-VI group of semiconductors compounds V.K. Singh et al. [1-3] and Bond length distortion in III-V group of semiconductor compounds Kalyan Singh et al. [4]. The ideas of simple force constant model suggested by Kraut and Harrison [5-8] have also described a method to estimate the local relaxation around impurities in semiconductors using just the natural bond length. In this model the second neighbour relaxation of the nearest neighbours. Thus the bond length distortion □d due to the size difference between the impurity and host atom in any defect system is given as three fourths the difference of the natural bond length of impurity-host and host-host bond.

$$\square d = 3/4\ (d_{\text{impurity-host}} - d_{\text{host-host}}) \qquad \ldots. (1)$$

The positive distortion + □d corresponds to the nearest neighbours relaxing outwards and the negative distortion - □d corresponds to the nearest neighbour relaxing inwards.

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

(i) Change in covalent energy of the host impurity bond with respect to that of host-host bond. The covalent energy V_2, which is the potential parameter in related with the bond length by the following equation.

$$d^2 = \left(\frac{24.532}{V_2}\right) \qquad \ldots.(2)$$

The polar energy V_3, is related with the bond length by following equation.

$$d = \left(\frac{8.163}{(K^2 \bar{\epsilon}_h^{-2} - 4V_3^2)^{1/4}}\right) \qquad \ldots. (3)$$

$\bar{\epsilon}_h$ Where K is an empirical parameters and is the cation-anion average hybrid energy and is given as

$$\bar{\epsilon}_h = \frac{1}{8}(n_c \epsilon_h^c + n_a \epsilon_h^a)$$

Where n_c and n_a are the number of electrons associated with the cation and anion respectively which participate in the bonds such as $n_c = 2$ and $n_a = 6$ for II-VI group of semiconductors.

(ii) The difference in electro-negativity (□□*) Between the host and that of the impurity atom.

(3) The change in covalency (□□$_c$) of the bond when the impurity replaces the host.

The covalent energy V_2 of the host-impurity bond for Be-Series, Zn-Series and Cd-Series of II-VI group of semi conductors are reported in table-1 and the rest input data for host compounds are taken from table-1 we have used the values of $d_{host-host}$ calculated by us in table- 2

$\bar{\epsilon}_h$ Table-1. The values of bond orbital parameters (V_2, V_3) covalency □$_c$, empirical parameter (k) and cation and anion average hybrid energy ()

Compound	V_2 (ev)	V_3 (ev)	□$_c$	k	$\bar{\epsilon}_h$
BeS	-6.360	-	0.98	-	-
BeSe	-5.860	-	0.95	-	-
BeTe	-4.920	-	1.00	-	-
ZnS	-4.510	4.13	0.68	1.39	10.83
ZnSe	-4.140	3.80	0.69	1.33	10.32
ZnTe	-3.430	3.04	0.69	1.22	9.20
CdS	-4.110	4.22	0.64	1.275	10.79
CdSe	-3.770	3.88	0.64	1.22	10.28
CdTe	-3.120	3.13	0.65	1.12	9.15

Table-2. The value of bond length II-VI group of semiconductors

Compound	Present work		Expt. Values (A^o)
	Equation (2) (A^o)	Equation (3) (A^o)	
BeS	1.96	-	2.100
BeSe	2.05	-	2.200
BeTe	2.23	-	2.400
ZnS	2.33	2.30	2.341
ZnSe	2.43	2.41	2.455
ZnTe	2.67	2.66	2.642
CdS	2.44	2.48	2.526
CdSe	2.55	2.60	2.620
CdTe	2.80	2.87	2.805

Table-3. Bond length distortion of impurities in II-VI group of semiconductors

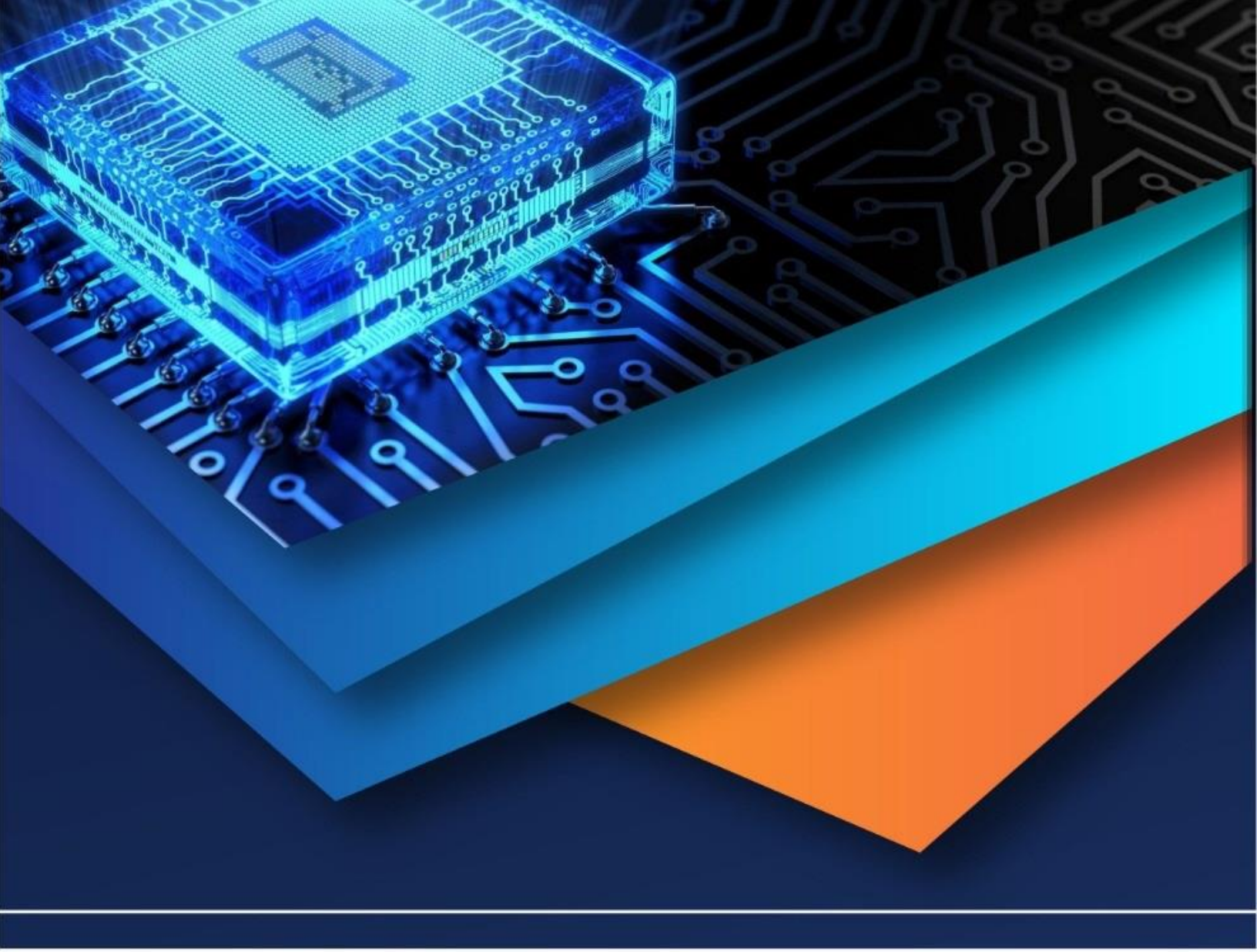
Compound	Impurity	V_2 (ev)	$d_{imp-host}$ (A^o)	□d (A^o)	Present work □d/d$_o$	Talwar □d/d$_o$
	Cd^c	-4.11	2.44	0.083	0.036	0.038
ZnS	Te^a	-3.43	2.67	0.225	0.109	0.085
	Cd^c	-3.77	2.55	0.090	0.037	0.037
ZnSe	Te^a	-3.43	2.67	0.180	0.074	0.053
	Cd^c	-3.12	2.80	0.098	0.037	0.038
ZnTe	Te^a	-4.14	2.40	-0.180	-0.067	-0.053

III. RESULT AND DISCUSSION

We have also studied the bond length distortion of atomic substitutions in III-V group of semiconductors [4]. Again we have studied bond length and bond length distortion of atomic substitutions in II-VI group of semiconductors. In every compound semi-conducting system the cationic substitution of groups II and III impurities is followed by the anionic substitution of groups V and VI impurities. We have studied the dependence of the sign and extent of bond length distortion of Cd cation and Te anion impurities in Zn-series as host system. We have calculated and reported the value of bond length (impurity-host system), bond length distortion and the ratio of bond length distortion to the host bond length in Table-3. It is found that the dependence of bond length and bond length distortion on bond orbital parameter V_2 is same as on the hybrid energy [9-11]. The sense of distortion is decided by the sign of the difference in electro-negativity between the host and the impurity atom. An impurity with a high electro-negativity than the host atom it is replacing, results in a contraction and vice-versa. This is an agreement with the suggestions made by Scheffler et al. [12, 13]. It is also suggested that when an impurity outer 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.

REFERENCES

[1] V.K. Singh, R.S. Indolia and Kalyan Singh, Acta Ciencia Indica Vol. XXXVI P, No. 2, 245 (2010).
[2] V.K. Singh, Manju Giri and Kalyan Singh, Acta Ciencia Indica Vol. XXXIX P, No. 3, 141 (2013)
[3] V.K. Singh, Manju Giri and Kalyan Singh, Acta Ciencia Indica Vol. XXXIX P, No. 3, 147 (2013).
[4] Kalyan Singh, P.K. Sharma, International Journal of Science and Research, Vol. 11, No. 5, 437 (2022).
[5] E.A. Kraut and W.A. Harrison, J.Vac. Sci. Technol. B **3**, 1267 (1985).
[6] W.A. Harrison, Electronic Structure and Properties of Solids (free man, San Francisco, 1980)
[7] W.A. Harrison, Phys. Rev. B **27**, 3592 (1983).
[8] W.A. Harrison, Phys. B **24**, 5835 (1981).
[9] D.N. Talwar, K.S. Suh and C.S. Ting, Phil Mag. B **54**, 93 (1986).
[10] D.N. Talwar, K.S. Suh and C.S. Ting, Phil Mag. B **56**, 593 (1987).
[11] S.G. Louie, Phys. Rev. B **22**, 1933 (1980).
[12] M. Scheffler, J.P. Vigneron and G.B. Bachelet, Phys. Rev. Lett. **49**, 1765 (1982).
[13] M. Scheffler, J.P. Vigneron and G.B. Bachelet, Phys. Rev. B **31**, 6541 (1985).



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