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RELATION OF LATTICE ENERGY WITH ELECTRONEGATIVITY AND PRINCIPAL QUANTUM NUMBER FOR TERNARY CHALCOPYRITE SEMI-CONDUCTORS

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Abstract

In this research paper, the lattice energy of $A^{I}B^{III}C_2^{VI}$ & $A^{II}B^{IV}C_2^{V}$ type chalcopyrite semi-conductors has been calculated. In this work, on the basis of chemical bond theory a new empirical relation has been developed between the lattice energy and the ratio of the principal quantum number and the electro-negativities of the constituent atoms of the ternary chalcopyrite compounds.

Keyword: Ternary Chalcopyrite Semiconductors, Lattice energy, Principal quantum number, Electro-negativity.

1.INTRODUCTION

Ternary chalcopyrites with the general formula $A^{I}B^{III}C_2^{VI}$ & $A^{II}B^{IV}C_2^{V}$ are of impressive intrigue in view of their potential optoelectronic applications as sun-powered converters, non-linear optical gadgets, light emitting diodes and finders. Their various forms are also utilized for the creation of indicators, lasers, and incorporated optic gadgets[1-29]. Notwithstanding their potential applications, versatile properties of I-III-VI_2 and II-IV-V_2 semi-conductors are as yet not adequately contemplated. The physico-mechanical properties, such as, lattice energy; bulk modulus, Plasmon energy and so forth of these semiconductors have been contemplated tentatively and hypothetically.
In the proposed relation just two parameters - electronegativity and principal quantum number of valence electrons in atoms framing the compounds are required as a contribution to compute lattice energy of ternary chalcopyrite semiconductors.

2.THEORY-

The lattice energy (crystal energy) of a crystalline solid may be defined as the energy released when ions are combined to form a compound. It is the proportion of the cohesive forces that bind crystals. There are very few researchers who worked for the lattice energy of binary and ternary chalcopyrites.

Reddy et. al[30] suggested a linear relation between lattice energy and Plasmon energy for binary compound semiconductors. The relation is as,

$$U = 381.9 + 24.3\ (\hbar w_p) \quad \text{.....(1)}$$

where U represents lattice energy and $\hbar w_p$ represents Plasmon energy of compounds.

Kumar et. al[31] proposed a quadratic relation between lattice energy and Plasmon energy for binary compound semiconductors as,

$$U = 421.224 + 27.940(\hbar w_p) - 0.178(\hbar w_p)^2 \quad \text{.....(2)}$$

Reddy et. al[32] proposed the following relation for the calculation of lattice energy,

$U = K_1 + K_2 e^{k_3 n} - K_4 e^{k_5 n}$ .....(3)

where K_1, K_2,K_3 and K_4 are constants.

Gorai et. al[33] proposed the relation,

$U = A + B(\hbar w_p)$.....(4)

where A and B are constants.

We have considered all the above relations proposed by various scientists for the estimation of lattice energy of binary chalcopyrite structure solids and propelled to investigate a new relation for the estimation of lattice energy of the ternary chalcopyrite solid. The greater part of the above relations require exceedingly complex component. In this exploration work, we have displayed an elective strategy for the estimation of lattice energy of ternary chalcopyrite structure solids which depends on just Microsoft-excel programming and logical calculation.

The above relations reveal that lattice energy of any material depends on the volume of its constituent atoms, Plasmon energy, refractive index, bond strength, bond length etc. The volume of the ternary chalcopyrite is related to its specific structure (Body center tetragonal). The deformation of the body center tetragonal structure is correlated with three lattice parameter a, c and u. These parameters are optimized through minimization of the total energy and accordingly lattice energy is estimated. The measurement of stiffness of the crystal is related to deformation produced in the crystal. The anisotropic strain of tetragonal structure is reflected by tetragonal deformation (2-c/a).This will also lead to a change in bond length which reveals anion displacement. This whole scenario will change the bond length and bond strength of the compounds. In order to take all these into account and to define the physico-mechanical property of ternary chalcopyrite solids, we have used two parameters - one parameter is the electronegativity which is the tendency of an atom to attract electrons towards itself during the formation of bonds, and another parameter is the principal quantum number. The longer the distance between the valence electrons and nuclei, the larger will be the principal quantum number. This would show larger electronic polarizability and hence higher lattice energy. Therefore, electronegativity and principal quantum number, both are assumed to be correlated with the nature of chemical bonding and predicting physico-mechanical property like lattice energy of ternary chalcopyrite structure solids. For ternary chalcopyrite structure solids, the lattice energy is assumed to be co-related to the contribution of three atoms A,B and C_2. Consider $\eta_{av} = \frac{(\eta_A+\eta_B+2\eta_C)^{1/4}}{4}$ be the average principal quantum number of the four constituents' atoms in ABC_2 ,then the lattice energy of ternary chalcopyrite semi-conductors can be expressed as-

$$U = a\left[\frac{\eta_{av}}{(\chi_A\chi_B)^{\frac{1}{4}}\ (\chi_C)^{1/2}}\right] + b \quad \text{.....(5)}$$

where a=117.24 , b=837.38 for I-III-VI_2 type semiconductors and a=355.5 , b=602.57 II-IV-V_2 type semi-conductors.

3.RESULTS AND DISCUSSION-

Using the above relation, we have calculated the values of lattice energy for I-III-VI_2 and II-IV-V_2 type ternary chalco-pyrite semiconductors and found the following results-

Table-1 : Lattice energy of I-III-VI_2 type chalcopyrite semiconductors-

Compounds	Value of $\frac{\eta_{av}}{(\chi_A\chi_B)^{\frac{1}{4}}\ (\chi_C)^{1/2}}$	Lattice energy (in electron volt)from relation (5)
$CuAlS_2$	0.53	899.51
$CuAlSe_2$	0.73	922.96
$CuAlTe_2$	1.11	967.51
$CuGaS_2$	0.57	904.20
$CuGaSe_2$	0.78	928.82

$CuGaTe_2$	1.18	975.72
$CuInS_2$	0.63	911.24
$CuInSe_2$	0.86	938.20
$CuInTe_2$	1.28	987.44
$AgAlS_2$	0.59	906.55
$AgAlSe_2$	0.80	931.17
$AgAlTe_2$	1.21	979.24
$AgGaS_2$	0.63	911.24
$AgGaSe_2$	0.85	937.03
$AgGaTe_2$	1.28	987.44
$AgInS_2$	0.69	918.27
$AgInSe_2$	0.93	946.41
$AgInTe_2$	1.39	1000.34

Table-2 : Lattice energy of II-IV-V_2 type chalcopyrite semiconductors-

Compounds	Value of $\frac{\eta_{av}}{(\chi_A\chi_B)^{\frac{1}{4}}\ (\chi_C)^{1/2}}$	Lattice energy (in electron volt) from relation (5)
$ZnSiP_2$	0.65	833.64
$ZnGeP_2$	0.71	854.97
$ZnSnP_2$	0.78	879.86
$ZnSiAs_2$	0.86	908.30
$ZnGeAs_2$	0.93	933.18
$ZnSnAs_2$	1.02	965.18
$CdSiP_2$	0.72	858.53
$CdGeP_2$	0.78	879.86
$CdSnP_2$	0.86	908.30
$CdSiAs_2$	0.95	940.29
$CdGeAs_2$	1.02	965.18
$CdSnAs_2$	1.11	997.17

For ternary chalcopyrite of I-III-VI_2 and II-IV-V_2 types, graphs has been plotted between the estimated values of Lattice energy and the ratio of average principal quantum number of atoms constituting compounds and electronegativity of atoms. Fig.1 shows the variation for of I-III-VI_2 and Fig.2 shows the variation for II-IV-V_2.

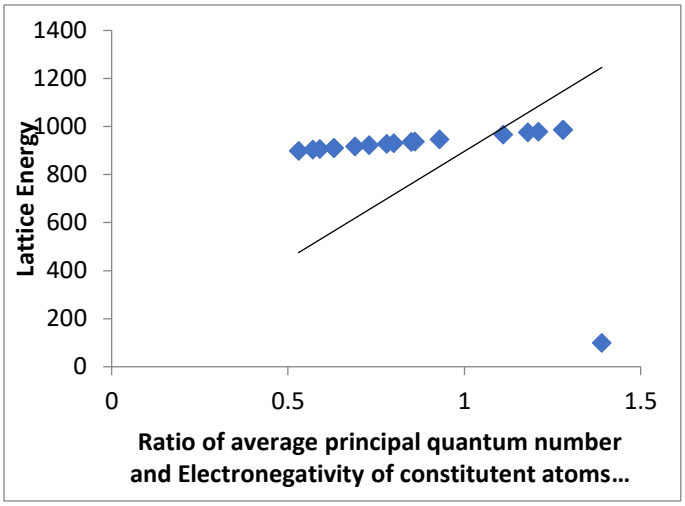

Fig.1: Plot of Lattice energy Vs Ratio of average principal quantum number and Electronegativity of constituent atoms of compounds for I-III-VI_2 .

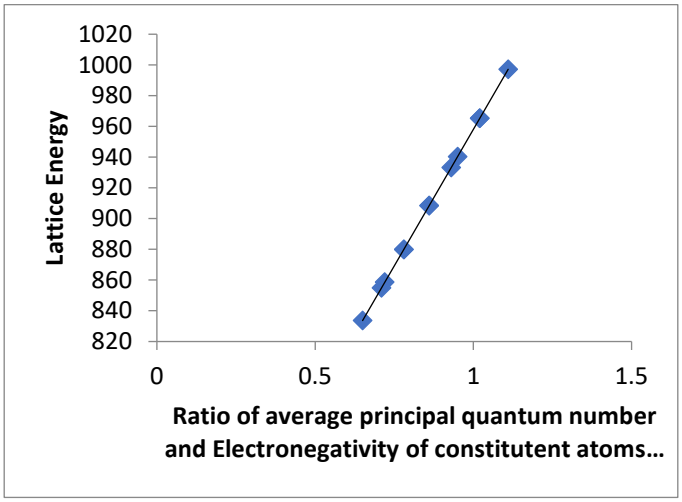

Fig.2: Plot of Lattice energy Vs Ratio of average principal quantum number and Electronegativity of constituent atoms of compounds for II-IV-V_2.

From the graphs it is clear that Lattice energy of ternary chalcopyrites varies linearly with the ratio of average principal quantum number and electronegativity of constituent atoms of compounds.

4.CONCLUSION

It is clear from the above calculations and graphs, that lattice energy of ternary chalcopyrite semiconductors depend on principal quantum number and electronegativity of compounds. The linear graphs validate our relation. So, the above relation can be used to determine the lattice energy of ternary chalcopyrite semiconductors. Also only the ratio of principal quantum number and electronegativity is required for the determination of lattice energy from the above relation. Thus the relation is simple one and less time consuming.

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