An Empirical Relation for the Calculation of Ionicity of Ternary Chalcopyrite Semi-Conductors

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***Abstract*- In this research paper, the ionicity of AIBIIIC2VI & AIIBIVC2V type chalcopyrite semi-conductors is calculated by using the high frequency di-electric constant data. On the basis of linear plot a new empirical relation has been developed between ionicity and high frequency di-electric constant of ternary chalcopyrite semi-conductors. The calculated values of ionicity are in close agreement with the experimental and the calculated values of different researchers.**

***Index Terms*- Ionicity, High frequency di-electric constant, Ternary Chalcopyrite Semiconductors.**

I INTRODUCTION

As ternary chalcopyrite semiconductors are derived from binary structures III-V and II-VI so they have high non-linear susceptibility. Also due to their anisotropic character, they are highly birefringence. High birefringence along with high non-linear susceptibility makes ternary chalcopyrite semiconductors very useful material for efficient second harmonic generation and phase matching. As ternary chalcopyrite semiconductors are applicable in the field of non-linear optics, light emitting diodes, solar cells, photovoltaic detectors, electronics etc. so numerous attempts have been made to understand their electronic, elastic, mechanical and optical properties1-5. Frequent attempts have been made to understand their crystal ionicity of ternary chalcopyrite semiconductors. Philips Van-Vechten6-8, Levine9, Amar et.al., Naresh et.al. and other researchers10-14 have developed various theories and calculated ionicity of semi-conductor compounds. In practice these theories require elaborate computation, and have been developed only for the limited semi-conductors.

Our proposed relation is only based on the value of high frequency di-electric constant so it turns out to be widely applicable.

II. THEORY

Naresh et.al[15]. proposed the relation for ionicity depending on di-electric constant as,

$$f_i = \sqrt{\frac{S_0}{\epsilon_\infty - 1}} \qquad (1)$$

where ε_∞ is the high frequency di-electric constant and S_0 is the constant having unity value.

Aman et.al[16]. derive the following relation,

$$f_i = Mr^n \qquad (2)$$

where M and n are constants and r is electron density parameter.

In this work, we have plotted the graph between known values of ionicity of ternary chalcopyrite semiconductors against their di-electric constants.

The variation of f_i Vs ε_∞ is shown in fig.1 for $A^IB^{III}C_2^{VI}$ and in fig.2 for $A^{II}B^{IV}C_2^{V}$. The graphs have been plotted using least square fitting method. From the graphs it is clear that f_i shows a linear relation with ε_∞ for both type of ternary chalcopyrite crystals.

From the graphs, we have expresses a relation between fi and ε_∞ for $A^IB^{III}C_2^{VI}$ as,

$$f_i = \alpha \in_\infty + \beta \quad \ldots \qquad (3)$$

where α =-0.1051, and β =1.15.

Again for $A^{II}B^{IV}C_2^{V,}$ we have expresses the relation between f_i and ε_∞ for $A^{II}B^{IV}C_2^{V}$ as,

$$f_i = \alpha \in_\infty + \beta \qquad (4)$$

where α =-0.0641,and β = 1.12.

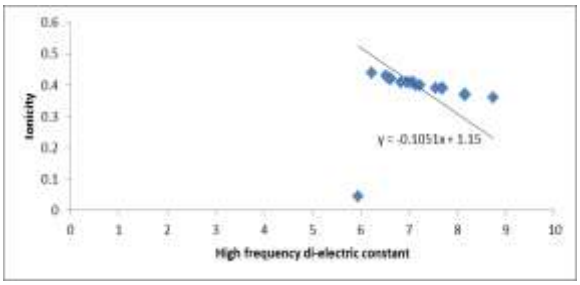

Fig.1: Plot of fi Vs ε∞ for I-III-VI2

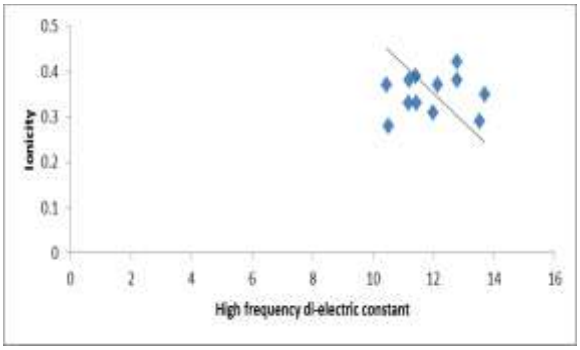

Fig.2: Plot of fi Vs ε∞ for II-IV-V2

III.RESULTS AND DISCUSSION

The fi of AIBIIIC2VI & AIIBIVC2V type chalcopyrite structure solids are estimated using equations 3 & 4. In table 1, the estimated values of fi for AIBIIIC2VI and in table 2 the estimated values of fi for AIIBIVC2V are listed along with the results of earlier researchers. It is observed that the calculated values are in better agreement with the other results.

Table-1: Crystal ionicity of I-III-VI2 type chalcopyrite semiconductors

Compounds	High frequency dielectric constant[17] ε_∞	Ionicity[18] (f_i)	Ionicity[15] (f_i)	Ionicity (f_i) [This Work]
$CuAlS_2$	5.95	0.69	0.45	0.52
$CuAlSe_2$	6.59	0.69	0.42	0.45
$CuAlTe_2$	7.55	0.71	0.39	0.35
$CuGaS_2$	6.23	0.69	0.44	0.49
$CuGaSe_2$	6.83	0.70	0.41	0.43
$CuGaTe_2$	7.67	0.71	0.39	0.34
$CuInS_2$	6.95	0.70	0.41	0.41
$CuInSe_2$	7.09	0.70	0.41	0.40
$CuInTe_2$	8.16	0.71	0.37	0.29
$AgAlS_2$	6.52	0.70	0.43	0.46
$AgAlSe_2$	7.13	0.70	0.40	0.40
$AgAlTe_2$	8.13	0.71	0.37	0.29
$AgGaS_2$	6.63	0.70	0.42	0.45
$AgGaSe_2$	7.22	0.70	0.40	0.39
$AgGaTe_2$	8.16	0.71	0.37	0.29
$AgInS_2$	7.03	0.70	0.41	0.41
$AgInSe_2$	7.70	0.71	0.39	0.34
$AgInTe_2$	8.74	0.72	0.36	0.23

Table-2: Crystal ionicity of II-IV-V2 type chalcopyrite semiconductors

Compounds	High frequency dielectric constant[17] ε_∞	Ionicity[18] (f_i)	Ionicity[15] (f_i)	Ionicity (f_i) [This Work]
$ZnSiP_2$	10.51	0.36	0.32	0.44
$ZnGeP_2$	11.18	0.36	0.31	0.40
$ZnSnP_2$	12.78	0.37	0.29	0.30
$ZnSiAs_2$	11.43	0.37	0.31	0.38
$ZnGeAs_2$	11.99	0.37	0.30	0.35
$ZnSnAs_2$	13.53	0.37	0.28	0.25
$CdSiP_2$	10.45	0.37	0.33	0.45
$CdGeP_2$	11.19	0.37	0.31	0.40
$CdSnP_2$	12.79	0.37	0.29	0.30
$CdSiAs_2$	11.41	0.37	0.31	0.38
$CdGeAs_2$	12.13	0.37	0.30	0.34
$CdSnAs_2$	13.69	0.37	0.28	0.24

IV. CONCLUSION

From the above results it is clear that just by knowing ε∞ one can easily determine the values of fi. The proposed relation yield not only satisfactory results but also a comparison with the standard data provides a direct and precise check of the validity. In the approach, the calculation is simple, fast and more accurate. The only information needed is ε∞, no other experimental values are required. It is natural to say that present approach can easily be extended to the other more complex crystals.

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