Research Journal of Recent Sciences _____ ISSN 2277-2502
Vol. **1(8),** 64-66, August **(2012)** *Res.J.Recent Sci.*

Short Communication

Electronic Properties of Ternary Compound Semiconductors

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Available online at: www.isca.in
Received 6th April 2012, revised 19th April 2012, accepted 25th April 2012

Abstract

The description of crystal ionicity developed by Phillips and Van Vechten has been successfully employed in a wide range of semi-conductors and insulators. However, the applicability of this Phillips and Van Vechten (PV) dielectric analysis has been limited to only the simple A^NB^{8-N} compounds, which contain only one type of bond. Levine has extended the theory of PV to multi bond and complex crystals. Levine's theory of ionicity has been used to calculate the various bond parameters for the chalcopyrites. In this paper a simple method based on the high frequency dielectric constants of solids, is proposed for the calculation of crystal ionicity (f_i) of chalcopyrite ($A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$) semiconductors. Our evaluated values are in excellent agreement with the values reported by different researchers.

Keywords: Crystal ionicity, dielectric constants, chalcopyrites.

Introduction

Structurally chalcopyrite compounds are derived from that of the binary sphalerite structure (III-V and II-VI) with a slight distortion. Therefore, like binary compounds they have a high non-linear susceptibility. However because of the presence of two types of bonds in chalcopyrites they become anisotropic. This anisotropy gives rise to high bifringence. High non-linear susceptibility coupled with high bifringence in these compounds makes them very useful for efficient second harmonic generation and phase matching. During the last few years[1-12], frequent attempts have been made to understand the electronic, mechanical, elastic and optical properties of chalcopyrite ($A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$) semiconductors. This is because of their interesting semi-conducting properties and various practical applications in the field of non-linear optics, electronics, photovoltaic detectors, light emitting diodes and solar cells etc. The concept of crystal ionicity of chemical bonding has been proved to be very useful in the characterization of molecular and solid state properties and there exist many ionicity scales proposed to correlate with a wide range of chemical and physical properties such as elastic constants, cohesive energy, heat of formation, bulk modulus, crystal structure etc[13].

Phillips and Van Vechten[14-16], Levine[13] and several other researchers[17-21] have developed various theories and calculated ionicity for the case of simple compounds. In practice these theories require elaborate computation, and have been developed only for the limited semiconductors. Therefore, we thought it would be of interest to give an alternative explanation for the crystal ionicity (f_i) in chalcopyrite ($A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$) semiconductors. In the proposed relation only one parameter such as the high frequency dielectric constant is required as input, to evaluate crystal ionicity of these compounds and the method turns out to be widely applicable.

Material and Methods

The average energy gap can be separated into the homopolar and the heteropolar parts according to the following relations[14-16]

$$E_g^2 = E_h^2 + E_c^2 \quad (1)$$

$$f_i = E_c^2 / E_g^2 \quad (2)$$

$$E_h^2 = 39.74 / d^{2.48} \quad (3)$$

$$E_c^2 = 14.4b \{(Z_A / r_o) - (n/m) \times (Z_B/r_o)\} e^{-K_s r_o} \quad (4)$$

Where E_g is the average energy gap of a crystal; f_i is the fractional ionicity; d is the nearest-neighbor distance (bond length), E_c the heteropolar part of average energy gap for A_mB_n compounds, b the pre-screening factor, $e^{-K_s r_o}$ the Thomas-Fermi screening factor, and r_o = d/2. The numerical factors in equations (3) and (4) and the following ones are given for d expressed in Å and energy in eV. The most generalized form of the above equations has been discussed by Levine [13] in detail. The equations given by Levine reduce to those of PV when only one type of bond is present in the crystal.

According to the Penn model[17], the average energy gaps (E_g) for a semiconductor is given by,

$$E_P = E_g = \hbar \omega_p \sqrt{\frac{S_o}{\varepsilon_\infty - 1}} \quad (E_p\text{=Penn gap}) \quad (5)$$

Where $\hbar\omega_p$ is the valence electron plasmon energy and S_0 is the quantity very near to unity and is responsible for the correction to bond model due to banding effect. The valence electron plasmon energy is given by[10],

$$\hbar\omega_p = 28.8\sqrt{\frac{n_{eff}\, d}{M}} \quad (6)$$

Where d and M are density and molecular or atomic mass respectively of material and n_{eff} is the effective number of valence electron. According to Tubb's[22], the crystal ionicity of a system is defined in terms of average energy gap E_g or Penn gap E_p and Plasmon energy gap $\hbar\omega_p$ by the following relation,

$$f_i = \frac{E_P}{\hbar\omega_p} = \frac{E_g}{\hbar\omega_P} \quad (7)$$

After solving the relations (5) and (7) crystal ionicity may be calculated by the following relation,

$$f_i = \sqrt{\frac{S_o}{\varepsilon_\infty - 1}} \quad (8)$$

Here ε_∞ is the high frequency dielectric constant. S_0 is the constant and equal to unity.

Results and Discussion

Using equation (8), crystal ionicity (f_i), for chalcopyrite ($A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$) semiconductors has been calculated. The results are presented in table 1 and 2. The calculated values are in fair agreement with the values reported by Levine[13] and V. Kumar[23-25].

Table-1
Values of crystal ionicity of $A^IB^{III}C_2^{VI}$ chalcopyrite semiconductors

Solids	ε_∞ [26]	f_i [27]	f_i [13]	f_i [This work]
$CuAlS_2$	5.95	0.69	00	0.45
$CuAlSe_2$	6.59	0.69	00	0.42
$CuAlTe_2$	7.55	0.71	00	0.39
$CuGaS_2$	6.23	0.69	0.70	0.44
$CuGaSe_2$	6.83	0.70	0.67	0.41
$CuGaTe_2$	7.67	0.71	00	0.39
$CuInS_2$	6.95	0.70	0.71	0.41
$CuInSe_2$	7.09	0.70	00	0.41
$CuInTe_2$	8.16	0.71	00	0.37
$AgAlS_2$	6.52	0.70	00	0.43
$AgAlSe_2$	7.13	0.70	00	0.40
$AgAlTe_2$	8.13	0.71	00	0.37
$AgGaS_2$	6.63	0.70	0.72	0.42
$AgGaSe_2$	7.22	0.70	0.71	0.40
$AgGaTe_2$	8.16	0.71	00	0.37
$AgInS_2$	7.03	0.70	00	0.41
$AgInSe_2$	7.7	0.71	0.73	0.39
$AgInTe_2$	8.74	0.72	00	0.36

Table-2
Values of crystal ionicity of $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors

Solids	ε_∞ [26]	f_i [27]	f_i [13]	f_i [This work]
$ZnSiP_2$	10.51	0.36	0.28	0.32
$ZnGeP_2$	11.18	0.36	0.33	0.31
$ZnSnP_2$	12.78	0.37	0.38	0.29
$ZnSiAs_2$	11.43	0.37	0.33	0.31
$ZnGeAs_2$	11.99	0.37	0.31	0.30
$ZnSnAs_2$	13.53	0.37	0.29	0.28
$CdSiP_2$	10.45	0.37	0.37	0.33
$CdGeP_2$	11.19	0.37	0.38	0.31
$CdSnP_2$	12.79	0.37	0.42	0.29
$CdSiAs_2$	11.41	0.37	0.39	0.31
$CdGeAs_2$	12.13	0.37	0.37	0.30
$CdSnAs_2$	13.69	0.37	0.35	0.28

Conclusion

The proposed empirical relation has been applied to evaluate crystal ionicity (f_i), of chalcopyrite ($A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$) semiconductors. We come to the conclusion that dielectric constanst of any compound is very important parameter for calculating the physical properties. It is also note worthy that the proposed relations are simpler widely applicable and values are in better agreement with reported data as compared to empirical relation proposed by previous researchers. The method presented in this work will be helpful to the material scientists for finding new materials with desired crystal ionicity (f_i), among the series of structurally similar materials.

Acknowledgement

One of the authors (Dr. Ajay Singh Verma, PH/08/0049) thankful to University Grant Commission, New Delhi, India, for supporting this research under the scheme of U. G. C. Dr. D. S. Kothari Post Doctoral Fellowship.

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