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Electronic Susceptibility of I-III-VI2 and II-IV-V2 type Ternary Chalcopyrite Semiconductors

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Abstract

In this paper a simple empirical formula for the calculation of electronic susceptibility of I-III-VI2 and II-IV-V2 type of ternary chalcopyrites has been proposed. The empirical relation is based on the plasma oscillation theory of solids. Values of electronic susceptibility calculated using the empirical formula show fairly good agreement with the experimental values and the values reported by earlier researchers.

Keywords: Ternary Chalcopyrites, Plasmon, Plasma Oscillation, Electronic Susceptibility

1. INTRODUCTION

I-III-VI2 and II-IV-V2 type of ternary chalcopyrites have attracted considerable attention because of their potential applications in electronic devices, non-linear optical devices, modulators, switches, converters, communication devices etc [1-10]. Their nano equivalents (Nano-ternary Chalcopyrites) are also used in different medical sectors even in present condition they are used in corona treatment. They are direct gap semiconducting compounds having tetragonal body centre structure. The structures of these ternary compounds are derived from their binary sphalerite structure and due to this they possess higher value of electronic susceptibility (non-linear susceptibility). The higher values of electronic susceptibility make them ideal material for phase matching devices and second harmonic generator.

Plasmon oscillations in metals, dielectrics or in semiconductors are the collective longitudinal excitations of the conduction electron gas. These oscillations are quantized and the quantum energy of these oscillations is known as Plasmon energy (hw_P). It has been well established that the Plasmon energy of metals or dielectrics change when they undergo chemical combinations with others to form compounds. This is due to the fact that the Plasmon energy depends on the effective number of valance electrons and the density of conduction electrons, which changes when a metal forms a compound [11]. We have calculated the electronic susceptibility of I-III-VI2 and II-IV-V2 type ternary chalcopyrite semiconductors using this concept.

Theory

From the free electron model, the Plasmon energy of a metal or a compound is given by,

$$E_p = h\sqrt{\frac{ne^2}{m\epsilon_0}} = hw_P \qquad (1)$$

where n is the conduction electron density, e is the elementary charge, m is the mass of electron, is the permittivity of free space, $\hbar$ is the reduced Planck constant and is the Plasmon frequency.

Equation (i) depends on fixed parameters which are independent on any physical factor so using Plasmon energy to calculate various optical or mechanical constants of ternary chalcopyrites is always beneficial.

Various researchers have proposed relations for calculation of non-linear susceptibility of ternary chalcopyrites. Verma et. al. [11] has proposed the relation for calculation of electronic susceptibility as,

$$\epsilon = \frac{500}{(hw_P)^v}$$

$$x = \varepsilon - 1 \qquad (2)$$

Here, V is a constant whose value is 1.45 for I-III-VI2 and 1.429 for II-IV-V2.

In the present work, we have plotted graphs between electric susceptibility and Plasmon energy of I-III-VI2 and II-IV-V2 type chalcopyrite semiconductors from their experimental values. Figures 1 and 2 shows the variation of electric susceptibility and Plasmon energy for both types of chalcopyrites. The graphs are linear in nature and R2 values are respectively 0.904 for I-III-VI2 and 0.8006 for II-IV-V2. From the graphs it is clear that electric susceptibility bears a linear relation with Plasmon energy in case of both type ternary chalcopyrite groups of compound.

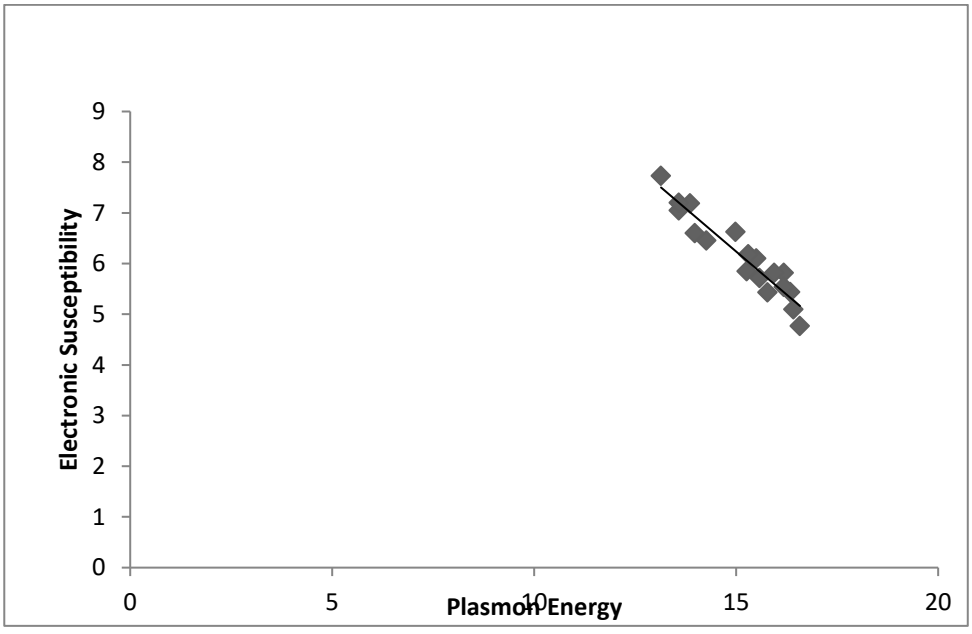

Fig 1 Variation of electronic susceptibility with Plasmon energy for I-III-VI2.

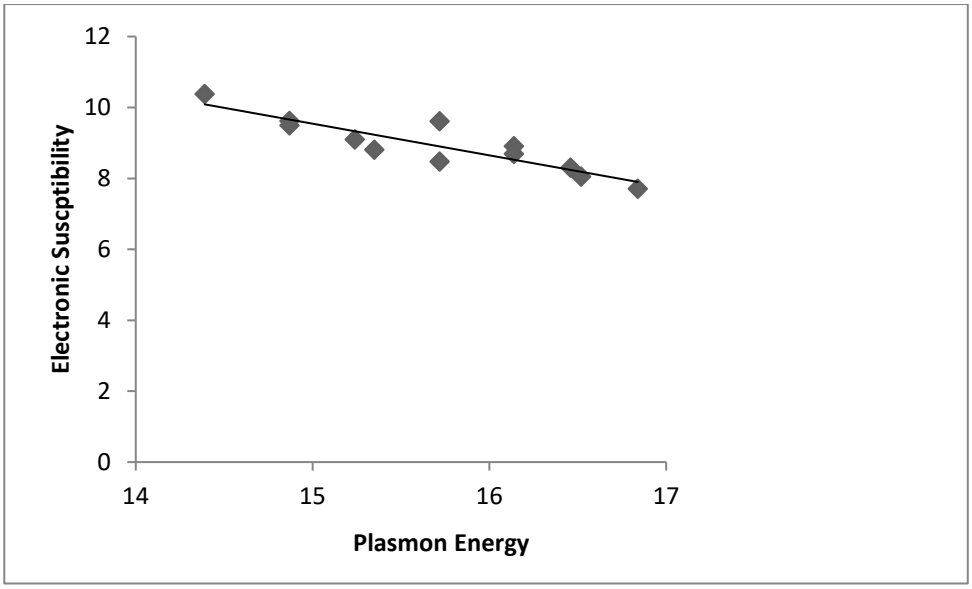

Fig 2 Variation of electronic susceptibility with Plasmon energy for II-IV-V2.

Using the nature of the graph, we have proposed the relation,

$$x = \alpha[h\omega_P] + \beta \qquad (3)$$

where α=-0.6797 and β=16.432 for I-III-VI2 and α=-0.8931 and β=22.939 for II-IV-VI2 type semiconductors.

Discussion and Conclusion

The values of electronic susceptibility of I-III-VI2 and II-IV-V2 types chalcopyrites are calculated using equation (iii) and the calculated values are listed in Tables 1 and 2 along with experimental values and values reported by other researchers.

Table-1: Electronic susceptibility of I-III-VI2 type chalcopyrite semiconductors

Compounds	**From equation (iii)**	**Ref.[11]**	**Ref.[12]**	**Experimental Value [1]**
$CuAlS_2$	5.16	4.769	4.768	5.2
$CuAlSe_2$	5.70	5.574	5.430	
$CuAlTe_2$	6.73	6.182	6.452	

$CuGaS_2$	5.27	4.866	5.094	
$CuGaSe_2$	5.84	5.705	5.716	
$CuGaTe_2$	6.92	6.628	6.597	
$CuInS_2$	5.43	5.680	5.816	5.4
$CuInSe_2$	6.05	6.237	5.851	
$CuInTe_2$	7.20	8.026	7.047	
$AgAlS_2$	5.32	4.483	5.437	5.3
$AgAlSe_2$	5.89	5.114	6.103	5.8
$AgAlTe_2$	7.01	6.211	7.188	
$AgGaS_2$	5.43	4.773	5.541	
$AgGaSe_2$	6.03	5.602	6.185	6.0
$AgGaTe_2$	7.20	6.626	7.200	
$AgInS_2$	5.59	5.324	5.918	
$AgInSe_2$	6.25	6.273	6.625	
$AgInTe_2$	7.50	7.494	7.731	7.5

Table-2

Electronic susceptibility of II-IV-V2 type chalcopyrite semiconductors

Compounds	**From equation (iii)**	**Ref.[11]**	**Experimental Value [1]**
$ZnSiP_2$	7.89	7.704	
$ZnGeP_2$	8.18	8.047	
$ZnSnP_2$	8.52	8.904	
$ZnSiAs_2$	8.89	8.473	
$ZnGeAs_2$	9.22	8.811	9.2
$ZnSnAs_2$	9.65	9.62	9.6
$CdSiP_2$	8.23	8.302	

$CdGeP_2$	8.52	8.694	
$CdSnP_2$	8.89	9.61	8.9
$CdSiAs_2$	9.32	9.10	
$CdGeAs_2$	9.65	9.49	
$CdSnAs_2$	10.08	10.38	

Fairly good agreement has been obtained between the calculated values and other reported values of electronic susceptibility of both types of ternary chalcopyrites. The percentage deviation of our calculated values from the experimental values lies in the range 0.05% to 1%.

The main advantage of the equation is its ease. It does not require any experimental data except the Plasmon energy.

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