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Electronic Polarizibility of Some Mixed I-III-VI_2 Chalcopyrites

P P Chandra
Assistant Professor,
Deptt. of Physics,
Banwarilal Bhalotia College,
Asansol, West Bengal

Abstract

Study on material parameters shows a simple correlation between electronegativity difference and lowest energy band gap for chalcopyrite semiconductors. Using the interrelationship among the electronic polarizibility, electronegativity difference and energy band gap values, compositional dependence of electronic polarizibility of some mixed I-III-VI_2chalcopyritecompounds have been evaluated and reported here.

Keywords: Chalcopyrite Compound, Electronic Polarizibility, Electronegativity Difference, Band Gap Energy

Introduction

Characterization and investigation of physical properties of multinary compounds are very important in the field of material science[1,2]. The chalcopyrite compounds and their mixed versions have shown their promise as technologically important materials for nonlinear frequency mixing devices, heterojunction solar cells and optoelectronic devices. The use of the mixed crystals by changing the composition and doping concentration has become a useful technique for different optoelectronic device design.As the band gap of the I-III-VI_2compounds covers a wide spectrum of electromagnetic wave, so they can be used as the basis for a variety of efficient light emitting devices. Further they are useful for applications as absorber for photovoltaic devices and in solar cells. They also provide unique optical, electrical and magnetic properties and show technological promise for a wide variety of optoelectronic applications [3, 4, 5, 6,7,8]like up conversion, down conversion and optical parametric oscillation producing tunable laser radiation, solar energy conversion, optical detectors and polycrystalline thin films. The search of the new compounds leads to the study of the mixed version of these types of compounds. The mixed version of I-III-VI_2compounds offer new possibilities for material engineering as their basic important parameters like lattice constant, band gap energy etc. can be controlled by changing the composition. Beside different design parameters like lowest energy band gap, refractive index, ionicity, thermal expansion coefficient, effective mass etc. electronic polarizibility is also very important. In this paper we have evaluated thisuseful parameteri.e. electronic polarizibility for some mixed chalcopyrite compounds for different compositions.

Aim of the Study

The mixed versions of the ternary chalcopyrite semiconductors belonging to I-III-VI_2have shown considerable possibilities for material engineering as their basic important parameters like lattice constant, band gap energy can be tailored to the desired value by changing the concentration.A good number of studies have been carried out on the crystal growth, band structure, dielectric, electrical, thermal dependence, pressure dependence and related parameters but sufficient interpretation of the measured data with the theory are not yet available for the compositional variation of the design parameters.In this connection we have studied in detail about some design parameters like band gap energy, optical electronegativity difference, electronic polarizibility of the I-III-VI_2 chalcopyrite compounds to find some interrelationship among them and using these correlations we have evaluated compositional variation of electronic polarizibility of the mixed chalcopyrite of the types$Cu/AgX_xX'_{1-x}Y_2$ and $Cu/AgX(Y_xY'_{1-x})_2$(X/X′ = Al, Ga, In and Y/Y′ = S, Se, Te).

Review of Literature

Electronic polarizibility of ions which plays an important role in determining the electrical properties of the semiconductor materials is strongly related to some optical properties like refractive index, dielectric constant etc. of the material. Therefore electronic polarizibility has been a matter of considerable importance for potential applications in integrated

optical devices. A number of investigations[9, 10, 11] are being carried out to evaluate the values of electronic polarizibility for this purpose. The refractive index is related to the lowest energy band gap of the material[12,13,14] which in turn has a strong correlation with another important parameter viz. optical electronegativity difference(Δχ). Duffy[15] found a correlation between energy band gap and optical electronegativity difference for various semiconductors through a relation given by E_g= 3.72 Δχ where $\Delta\chi = \Delta\chi_{anion} - \Delta\chi_{cation}$. Using various types of correlationship between different material parameters Moss[16] found a relation between refractive index(n) and optical electronegativity difference as $n = \left(\frac{25.54}{\Delta\chi}\right)^{\frac{1}{4}}$. Several types of correlations are proposed by the investigators between refractive index and optical electronegativity difference[10,17, 18]. Different theories have been proposed by the researchers to calculate electronic polarizibility and among themClausius- Mossoti relation which relates the electronic polarizibility with dielectric constant is famous one. Using these types of interrelationships of the material parameters Reddy et.al[11]proposed an expression for electronic polarizibility(α).

Now the mixed chalcopyrites compounds and even their nano crystals are getting considerable interest for potential applications in photovoltaic solar cells.[19, 20, 21, 22, 23]and other optoelectronic device applications.[24, 25]The advent of modern crystal growth techniques gave further impetus to the study and application of mixed crystals[26, 27, 28] as these compounds offer new possibilities for material engineering through the independent control of the important design parameters.

Concept and Hypothesis

As proposed by Reddy et.al. [11] electronic polarizibility of the semiconductor materials is given by $\alpha = 0.395\times10^{-24}\times\left(\frac{4.207+k}{7.207+k}\right)\frac{M}{\rho}$ ……(1)

where $k = \ln\Delta\chi\left(\ln\Delta\chi - 4.564\right)$, M is the molecular weight and ρ is the density of the substance.In this paper we have used interpolation schemes as a tool to estimatedensity and molecular weight of the mixed crystals represented by $Cu/AgX_xX'_{1-x}Y_2$ and $Cu/AgX(Y_xY'_{1-x})_2$. The density and molecular weight of the alloy can be obtained by interpolation from those of theconstituents $Cu/AgXY_2$ and $Cu/AgX'_{1-x}Y_2$ or$Cu/AgXY_2$and $Cu/AgXY'_2$using the relation $T_{ij} = xB_i + (1-x)B_j$ where B_i and B_j are the value of the parameter of the two constituent compounds.

Research design

Our study of different parameters of the I-III-VI_2semiconductors results in finding a strong correlation of the band gap energy with their molecular weight. It is interesting to find that band gap energy has aparabolic variation with the logarithm of the molecular weight. Our study also reveals that electronegativity difference (Δχ) is strongly correlated with lowest energy band gap(E_g) through a linear relationship of the form Δχ = A E_g + B for this group of materials where A and B are constants. The necessary data for electronegativity difference and lowest energy band gap are taken from different references.Using the correlation of energy band gap and molecular weight we have obtained the values of the lowest energy band gap for the different compositions of the mixed chalcopyrite compounds and then values of electronegativity difference for those crystals have been evaluated using the correlation of electronegativity difference with lowest energy band gap. Ultimately electronic polarizibility of these mixed crystals for different composition has been evaluated byequation (1).

Findings

In this paper, we present some important correlations between various material parameters for the I-III-VI_2 semiconductors. In figure 1 and figure 2 we have plotted the variation of optical electronegativity differences with energy band gap for Cu and Ag as the noble metals respectively. These plots shows a linear relationship between the two parameters of the formΔχ = A E_g + B where A and B are two constants and have different values for Cu compounds and Ag compounds. Our study also have found a parabolic correlation of energy band gap with the logarithm of molecular weight of the I-III-VI_2 semiconductors and thesehas been represented in figure 3 and figure 4 respectively for Cu and Ag compounds.The variations of electronic polarizibility with concentration for different mixedI-III-VI_2 compounds with Cu as group- I element have been shown in figures 5(a) to 5(d) and with Ag as group- I elementin figures 6(a) to 6(d) respectively.

Figure 1 Variation of optical electronegativity with band gap energy for Cu chalcopyrites

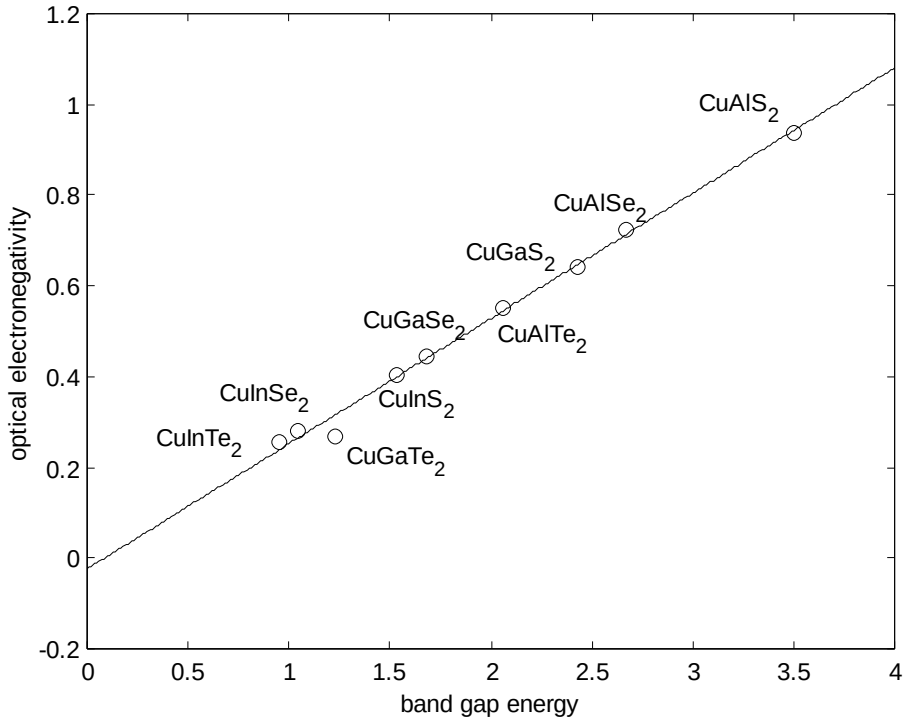


Figure 2. Variation of optical electronegativity with band gap energy for Ag chalcopyrites

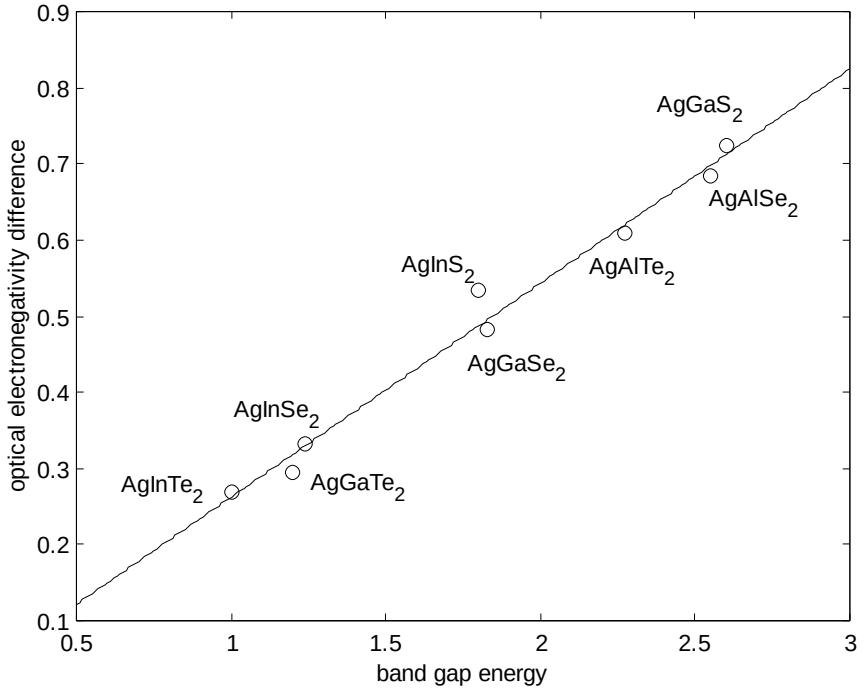


Figure 3. Variation of band gap energy with logarithm of molecular weight for Cu chalcopyrites

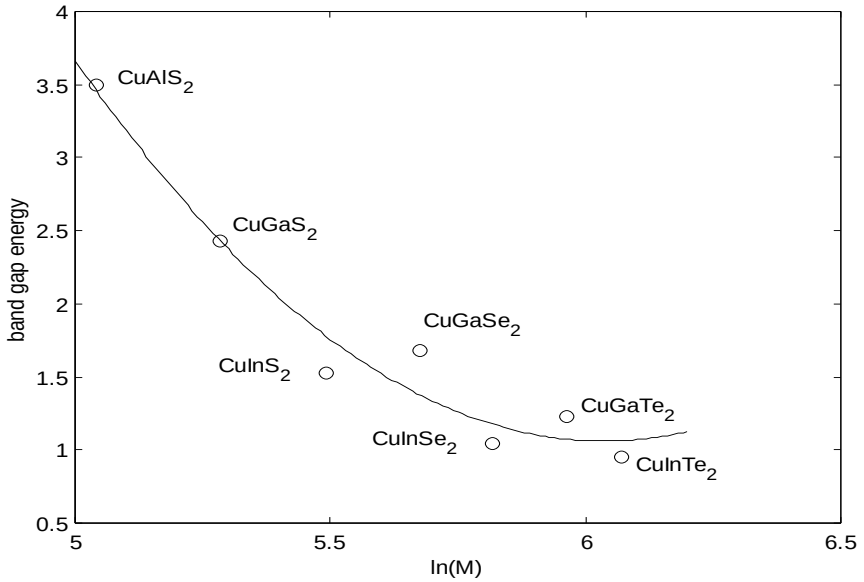


Figure 4. Variation of band gap energy with logarithm of molecular weight for Ag chalcopyrites

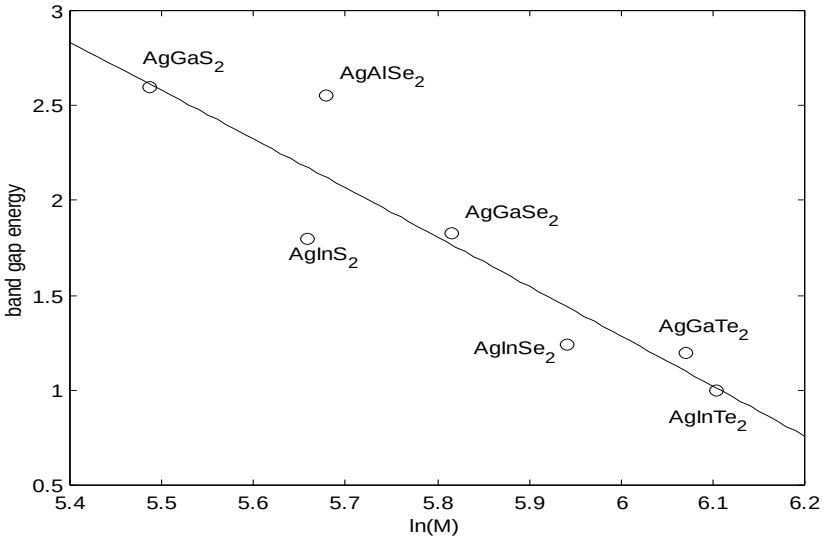


Figure 5(a)

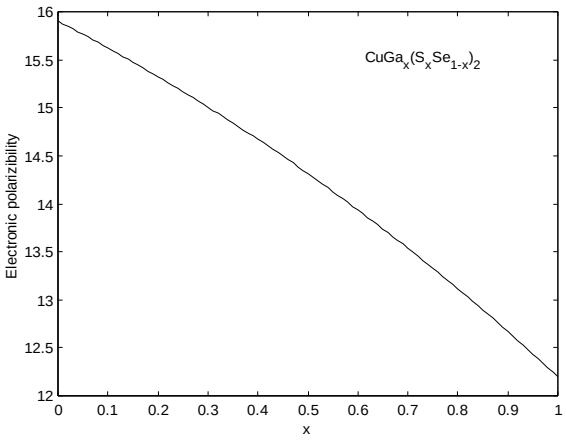


Figure 5(b)

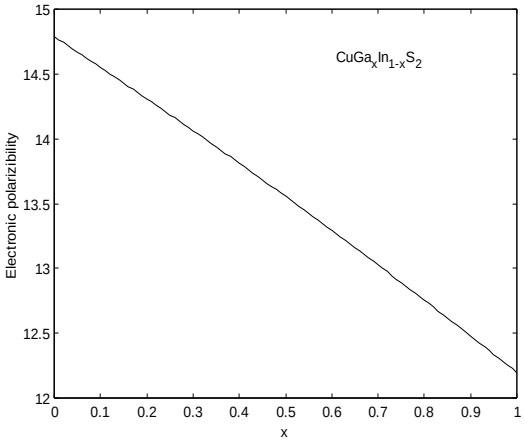


Figure 5(c)

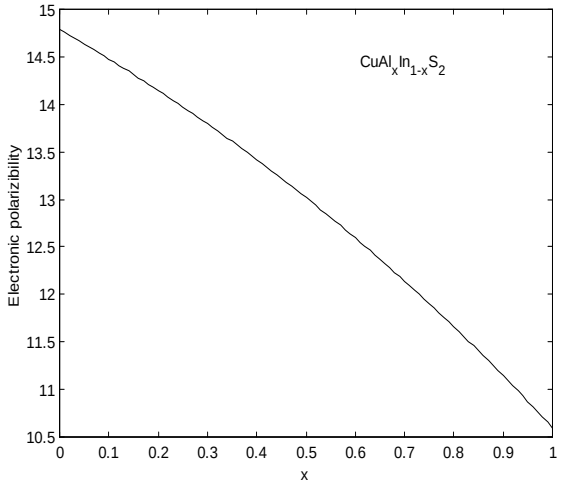


Figure 5(d)

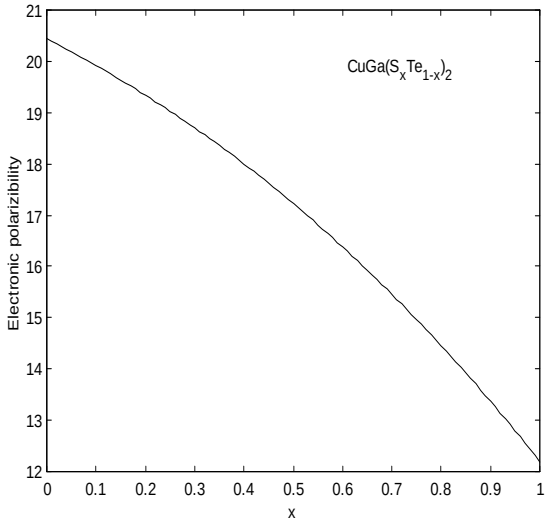


Figure 6(a)

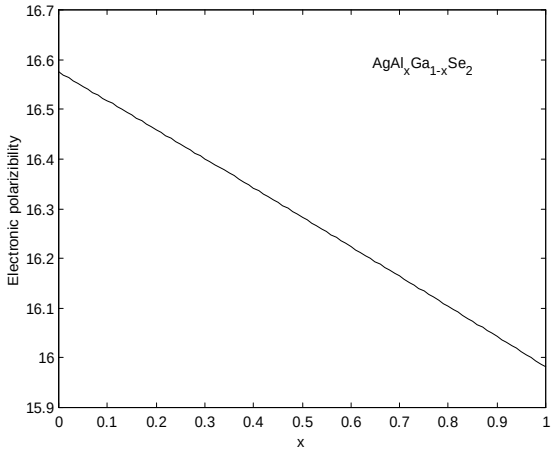


Figure 6(b)

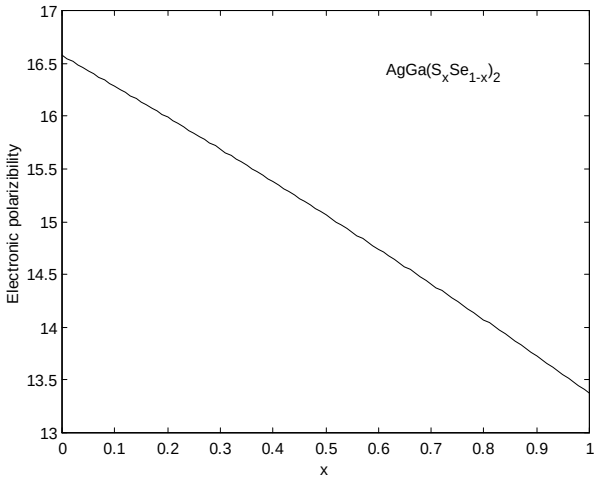


Figure 6(c)

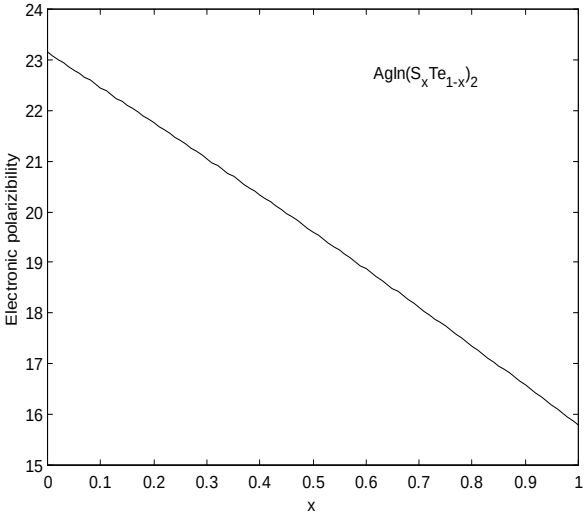
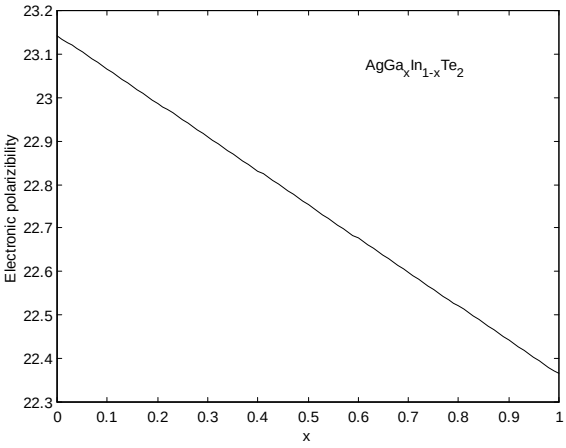


Figure 6(d)



Conclusion

Detailed knowledge of electronic polarizibility of the mixed chalcopyrite crystals for different concentrationwillbe very much helpful for selectionof the particular material for specific device design. Different correlation among the different material parameters presented here will also be helpful for finding different material parameters. Knowledge gained from such studies would undoubtedly help not only to get good quality of crystals but also to realize new combinations of semiconductor materials for various device design applications.

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