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On Some Important Material Parameters of Some III-V and II-VI Quaternary Compounds Relevant to Device Design

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Abstract

Different studies have shown that bond length is related to the number of valence electrons and hence the Plasmon energy indicating that there must be some interrelationship between the energy gap, dielectric constant and the Plasmon energy and some relations of E_h (homopolar part of energy band gap), E_c (heteropolar part of energy band gap), E_g (energy band gap), ε (dielectric constant) and f_i (Phillip's ionicity) with Plasmon energy for the III-V, II-VI and I-VII binary materials have been proposed. Using these different studies we have reported here the values of dielectric constant and Phillip's ionicity for some quaternary III-V and II-VI compounds and compared the values obtained from different approaches.

Keywords: Mixed Semiconductors, Dielectric Constant, Phillips Ionicity, Plasmon Energy.

Introduction

In this paper we have studied quaternary compounds like AlGaPAs, AlGaAsSb, AlInPSb, AlInPAs, GaInPAs, GaInAsSb, ZnCdSSe, ZnCdSTe, ZnCdSeTe, MgZnSSe etc. and reported the values of the Phillip's ionicity, complex band gap dielectric constant etc. for the mixed III-V and II-VI compounds mentioned above. Again choice of suitable substrate to grow good quality crystals is very important. We have also studied about the lattice matching condition on different substrates for different quaternary compounds which in turn would help to choose the right substrate for growing of crystal for specific design.

Objective of the Study

Quaternary alloys offer new possibilities for material engineering as their basic important parameters like lattice constant, band gap energy and valence band offset can be controlled independently. The quaternary III-V and II-VI compounds are getting considerable interest because they may give access to lattice matching with other II-VI or III-V semiconductors along with controllable band gap for potential applications in optoelectronics and photovoltaic solar cells. The reduction of the lattice mismatch may be obtained by graded layers of mixed crystals. Thus growth and characterization of the compound semiconductors are playing an important role in modern material science. In heteroepitaxy, when materials are deposited on a substrate with a different lattice constant normally a strain is induced. If the grown crystal has a larger lattice constant than the substrate a compressive strain is generated in the grown crystal while with a smaller lattice constant the atoms are pulled apart to accommodate the substrate, forming a tensile strain. We have evaluated the values of Phillip's ionicity and dielectric constant of the quaternary compounds taking in to account the lattice matching conditions of the crystals on different substrates.

Review of Literature

In the recent years, technological interest in alloys arises for possibilities to develop semiconductors of adjustable energy gap and dielectric constant. The wavelength region 1-2 μm [1,2,3,4,5] is very useful for optoelectronic devices particularly for optical communication because of the presence of minimum loss at 1.5μm [6,7,8,9] and minimum dispersion at 1.3μm in optical fiber. The spectral region 2-4μm is drawing considerable attention because of recent development of low loss fluoride glass fibers in this spectral region and λ = 800 nm is useful for communication, entertainment and medical applications. And around this wavelength high powered devices have been built. Not only the single

crystal, the mixed compound semiconductors are coming out as important materials as the design parameters like lowest energy band gap, lattice parameter, thermal expansion coefficient and band structure parameter can be tailored to the desired values by changing the concentration of the constituent components of the crystal. As the material selection for device applications [9] is limited within III-V and II-VI compounds, several kinds of ternary and quaternary compounds are being considered. But the selection of the materials depends among other factors, on the quality of the crystals and easiness of the crystal growth. Thus growth, characterization and investigation of physical properties of ternary and multinary compounds play an important role in the field of material research and their applications. In the recent years, technological interest have been shown in the optical devices that can operate in the wide spectrum range which motivated research work in III-V and II-VI [10,11] materials and their mixed versions for the development of new semiconductor materials. The broad range of band gaps of the III-V and II-VI semiconductors play a key role to make study on them. Most of the III-V and II-VI semiconductors have direct band gap along with a high optical absorption and emission coefficients. As the band gap of these compounds covers the spectrum from ultraviolet to infrared, so can be 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. The search of the new compounds leads to the study from the binary to multinary alloys.

Concept and Hypothesis

Different researchers have studied various electronic and optical properties of III-V and II-VI compounds. Most of the models proposed by different researchers require experimental data for some parameters to evaluate the optical and electronic properties. But many of these compounds are very recently formed and so sufficient experimental data are not available for them. Recently the researchers have developed number of models to evaluate various properties of solids based on the theory of Plasmon oscillation which is related to the effective number of valence electrons in a semiconductor. Phillips and Van Vetchen have shown the dependence of bond length on the number of valence electrons and so it is expected that energy band gap, dielectric constant, ionicity of the materials should have some dependence on the number of valence electrons. The Plasmon energy ($\hbar\omega_p$) shows dependence on the number of valence electrons (Z) through the relation $\hbar\omega_p = 28.8\sqrt{\frac{Z\rho}{M}}$, where ρ is density and M is the molecular weight. Kumar et.al.[12] gave a simple relation of Phillips ionicity and dielectric constant of III-V and II-VI binary compounds as

$f_i = C_1 - C_2(\hbar\omega_p)$, $\varepsilon = C_3 - C_4(\hbar\omega_p)$

where C_1, C_2, C_3 and C_4 takes values as 0.6501, 0.0011, 10.7874, 0.2546 for II-VI compounds and 0.1809, -0.0126, 24.9501, 0.9350 for III-V compounds respectively. We extend these theories of the binary compounds to ternary any more complex compounds formed from these groups to evaluate the values of the parameters of the mixed crystals.

Research Design

In this paper quaternary compounds have been represented by $A_{1-x}B_xC_{1-y}D_y$ where *A* & *B* are groupII/III elements (between *A* and *B*, *A* has lower atomic number) and *C* & *D* are groupV/VI elements (between *C* and *D*, *C* has lower atomic number). A quaternary alloy parameter is described by *Q(x,y)* over *x, y* composition *(0≤x≤1, 0≤y≤1)* which along with *x* and *y* forms a three dimensional surface with values of the parameter for different compositions. The four corners of the surface gives the value of the parameter for four binaries *AC (x =1, y = 0), AD (x = 1, y = 1), BC (x = 0, y = 0)* and *BD (x = 0, y = 1)*. Similarly the four boundaries of the surface give the variation of the parameter with composition for the ternaries $AC_{1-y}D_y$ *(x = 1),* $BC_{1-y}D_y$ *(x = 0),* $A_xB_{1-x}C$ *(y =0)* and $A_xB_{1-x}D$ *(y = 1)*. If the parameter of the four constituent binaries of a quaternary compound are known, we can use the well known interpolation schemes

$$Q(x,y) = (1-x)[yB_{AC} + (1-y)B_{AD}] + x[yB_{BC} + (1-y)B_{BD}]. \quad \text{.....(1)}$$

$$Q(x,y) = \frac{x(1-x)[(1-y)T_{ABD} + yT_{ABC}] + y(1-y)[(1-x)T_{ACD} + xT_{BCD}]}{x(1-x) + y(1-y)} \quad \text{..... (2)}$$

Findings

Table 1 shows lattice matching conditions for some quaternary III-V and II-VI crystals on different substrates. In the figure 1(a) and 1(b) compositional variation of Phillips ionicity of ZnCdSSe and GaInAsSb have been plotted for the region *0≤x≤1, 0≤y≤1* along with the variation of the same under lattice matching condition (black solid line) using GaSb substrate. Figure 2(a) to 2(e) represents the values of the Phillips ionicity of the quaternary compounds for different compositions on different substrates and figure 3(a) to 3(e) shows the variation of dielectric constant of the quaternary compounds with composition on different substrates. We have compared the results obtained in this study with those obtained from interpolation methods and the agreement is good. One such comparison has been shown in table 2.

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Fig 1(a)

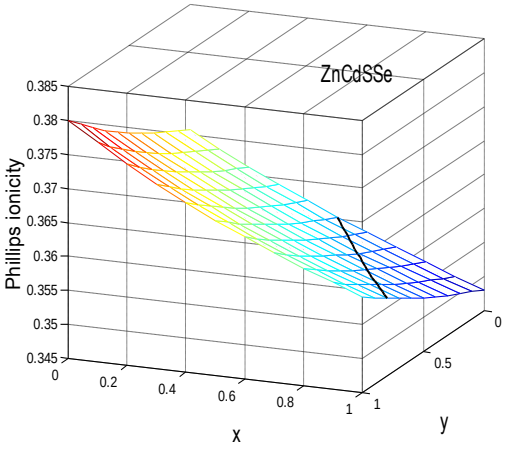


Fig 1(b)

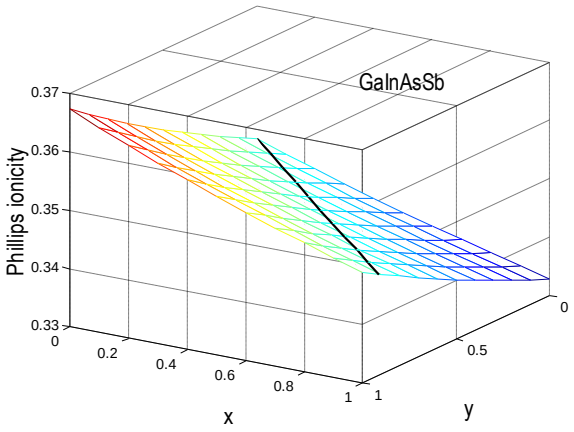


Table 1 : Lattice Matching Conditions of Some Mixed Crystals on Different Substrates

Compound	Substrates	Lattice Matching Condition	Compositional Range
$Al_{1-x}In_xP_ySb_{1-y}$	GaAs	$y = \frac{0.48 + 0.344x}{0.67 - 0.063x}$	0.715 ≤ y ≤ 1 0 ≤ x ≤ 0.47
	InAs	$y = \frac{0.08 + 0.344x}{0.67 - 0.063x}$	0.114 ≤y ≤ 0.689 0 ≤ x ≤ 1
$Al_{1-x}In_xAs_ySb_{1-y}$	GaSb	$y = \frac{0.04 + 0.3437x}{0.475 - 0.0543x}$	0.085 ≤ y ≤ 0.91 0 ≤ x ≤ 1
	InP	$y = \frac{0.27 + 0.344x}{0.47 - 0.054x}$	0.56 ≤ y ≤ 1 0 ≤ x ≤ 0.52
$Zn_{1-x}Cd_xS_ySe_{1-y}$	InP	$y = \frac{0.4x - 0.2}{0.26 - 0.01x}$	0.5<x<1 0<y<0.8
	CdS	$y = \frac{0.4x - 0.15}{0.26 - 0.01x}$	0.375<x<1 0<y<1
$Zn_{1-x}Cd_xS_{ey}Te_{1-y}$	ZnTe	$y = \frac{0.472x}{0.339 + 0.133x}$	0<x<1 0<y<0.99
	GaSb	$y = \frac{0.08 + 0.472x}{0.339 + 0.133x}$	0<x<0.75 0.24<y<1

Table 2: Comparison of Values of Phillips Ionicity Obtained from Different Methods

$Al_{1-x}In_xAs_{1-y}Sb_y$ on InP		
Concentration	**Value of Phillips Ionicity from This Study**	**Value of Phillips Ionicity from Interpolation Method**
x=0.5	0.3453	0.2997
x= 0.6	0.3454	0.3100
x=0.7	0.3457	0.3205
x=0.8	0.3461	0.3313
x=0.9	0.3466	0.3424
x=1.0	0.3473	0.3538

Fig 2(a)

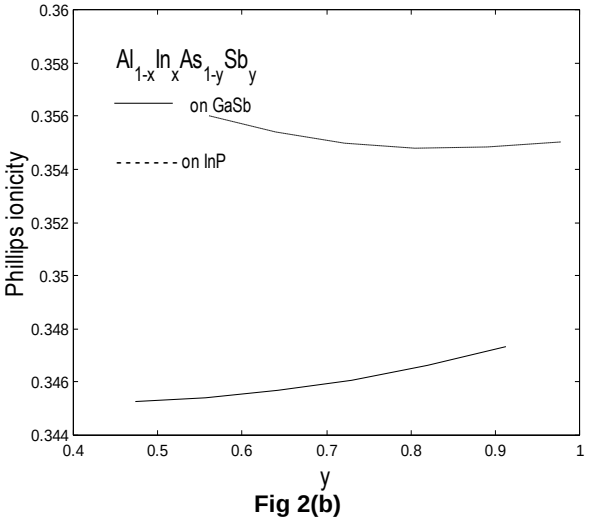


Fig 2(b)

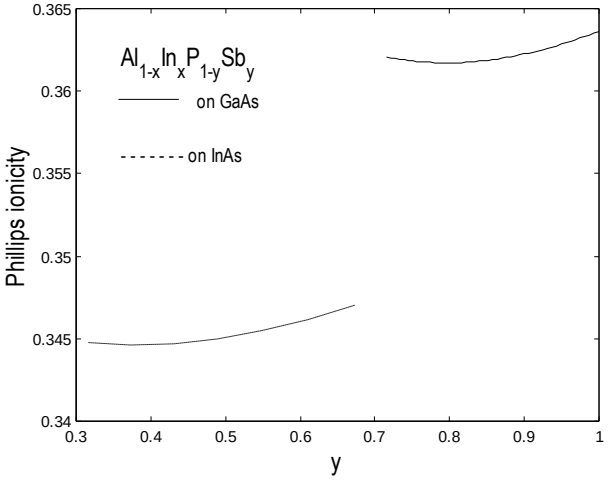


Fig 2(c)

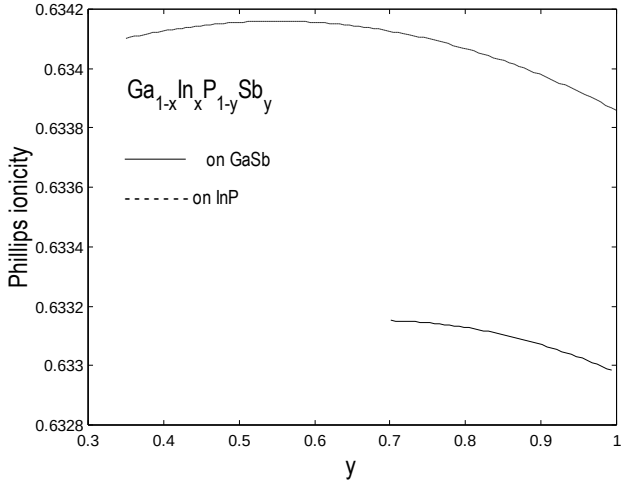


Fig 2(d)

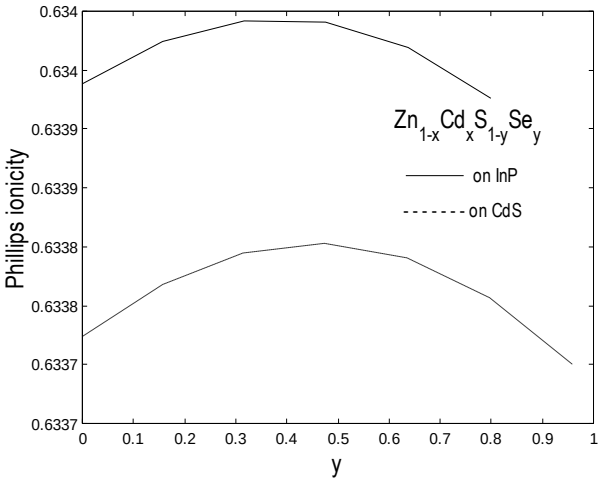


Fig 2(e)

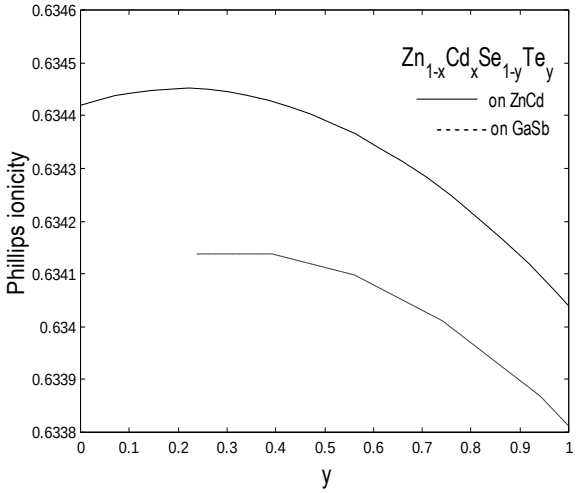


Fig 3(a)

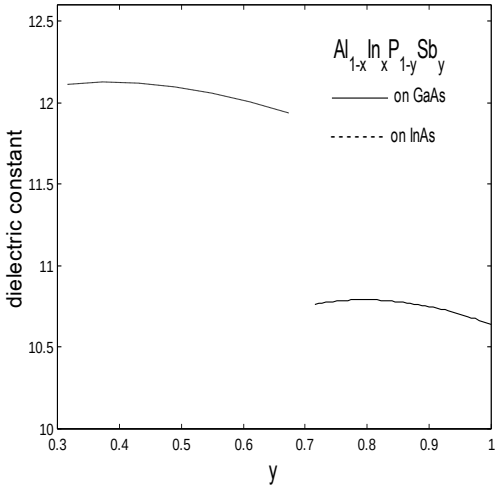


Fig 3(b)

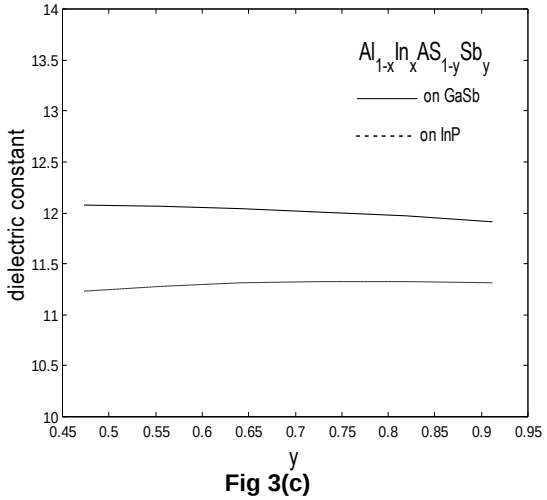
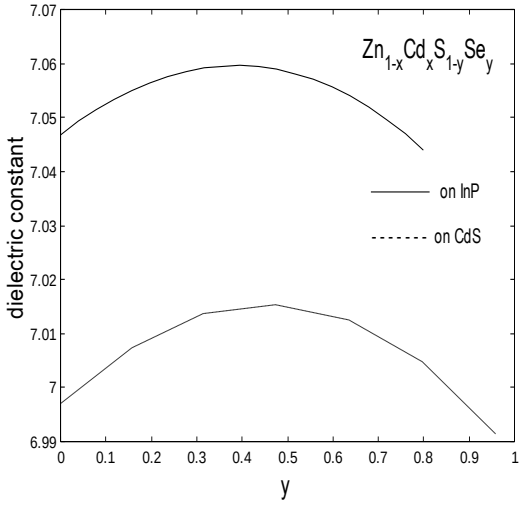


Fig 3(c)



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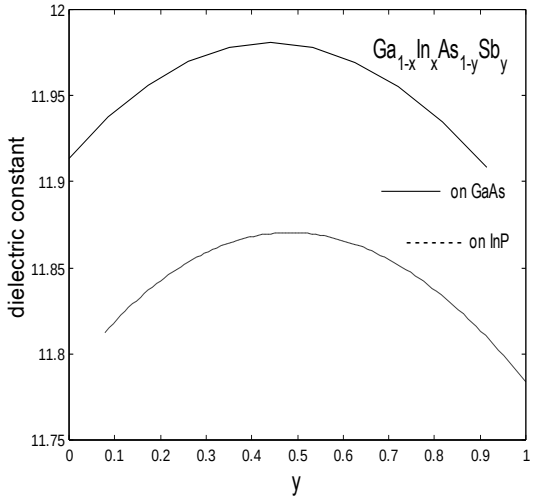
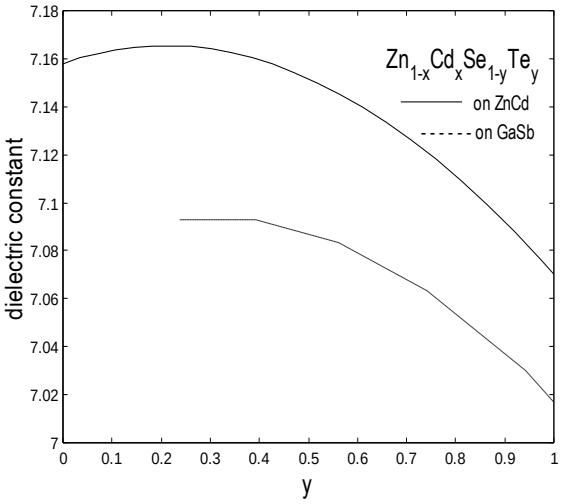


Fig 3(e)



Conclusion

A detailed study of Phillips ionicity and dielectric constant for various combinations of III-V and II-VI quaternary compounds have been presented in this paper where the evaluations have been done considering only those compositions of the crystals for which the crystal can be grown on a suitable substrate. Analysis of the result shows that the results obtained from the two methods are closely matched and thus support the methods to evaluate the values of different parameters for mixed crystals at different compositions. Detailed knowledge of Phillips ionicity and dielectric constant of the mixed crystals will be very much helpful for the material preparation, ie, the growth of particular material for specific device design and knowledge gained from such studies would undoubtedly help to grow good quality of crystals for various device design applications.

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