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THEORETICAL STUDY ON THE ELECTRICAL PROPERTIES OF SOME III-V AND IV-IV COMPOUNDS

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A theoretical Study on GaX, InX (X=As, P and Sb), $Al_xGa_{1-x}As$, $Ga_xIn_{1-x}Sb$ and Si_xGe_{1-x} has been made for deducing electrical transport properties using only two parameters, namely lattice constant and activation energy. The calculated electrical properties electrical resistivity, carrier mobility, carrier concentration, carrier effective mass and dielectric constant are compared with the available experimental results. They are found to be in good agreement with each other. Then, the limitation of this theoretical study has also been discussed in this paper.

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1. Introduction

Semiconducting materials basically have structures depending on the nature of bonding. They have tetrahedral bonds and therefore form cubic or hexagonal structures. Elemental semiconductors such as Si and Ge have diamond structures. Each atom has tetrahedral bondings with each other due to sp^3 hybrid orbitals. Compound semiconductors such as GaX, InX (X=As, P and Sb) have zinc blende structures which is similar to diamond structures [1,2]. The compound semiconductors have tetrahedral bonds but they include not only covalent bonds but also ionic bonds. Because, the compounds are formed from different ionic electronegativity. The difference of electronegativity indicates the strength with which the atoms attract electrons. The difference of electro negativity of constituent element is therefore an indication of the ionic strength. When the ionicity is strong, constituent elements are strongly attracted[2]. The compound semiconductors consisting of various elements have wide range of physical properties. The physical properties which may vary, include band gaps, crystal lattice structures, electron and hole mobilities, optical properties, thermal conductivity and so on. Considerable information is now becoming available on the physical properties but in many case the data is limited. It is very important to understand the physical properties and therefore requires more investigations. So, in this paper an attempt of theoretical study has been carried out on the following systems on GaX, InX (X=As, P and Sb), $Al_xGa_{1-x}As$, $Ga_xIn_{1-x}Sb$ and Si_xGe_{1-x} and the results are compared with the experimental results.

2. Theory

Compound semiconductor materials can be predicted by a simple rule. When the total number of valance electrons of constituent elements are divided by the number of elements comprising the compound and when this ratio gives four, the compound has a tendency to be semiconducting [1,2]. There are various semiconductor materials such as elemental, II-VI, III-V, IV-IV, and V-VI compounds. Among these the present theoretical study has been carried out on

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III-V compounds on GaX, InX (X=As, P and Sb), and IV-IV compound Si_xGe_{1-x}. The study has been extended to some ternary systems $Al_xGa_{1-x}As$ and $Ga_xIn_{1-x}Sb$.

The electrical conductivity σ can be calculated [3,4] by using the formula

$$\sigma = neu = \frac{1}{\rho} \tag{1}$$

where n is the carrier concentration, e is the electronic charge, u is the carrier mobility and ρ is the electrical resistivity.

The carrier concentration n can be calculated [5] from the carrier effective mass m* and activation energy ΔE by the expression

$$n = \frac{2(2\pi m^* kT)^{3/2}}{h^3} \exp\left(-\frac{\Delta E}{2kT}\right) \tag{2}$$

where k is the Boltzman's constant, h is the Plank's constant and T is the temperature.

The effective mass m* can be given [6] in terms of lattice parameter and a activation energy ΔE as

$$\frac{m_0}{m^*} = 1 + \frac{2\lambda^2}{m_0 a^2 \Delta E} \tag{3}$$

where m_0 is the electron rest mass and $\lambda^2 = \hbar^2$.

The electron mobility [7] is determined by using the formula,

$$u = \frac{3\varepsilon^2}{16\pi^2 m^* \left[\ln(1+x) - \frac{x}{1+x}\right]} \left(\frac{h}{e}\right)^3 \tag{4}$$

The value of x is calculated by the formula

$$x = \left(\frac{h}{e}\right)^2 \left(\frac{e}{m^*}\right) \left(\frac{3N}{8\pi}\right)^{1/3}$$

where N represents the impurity concentration which is given by

$$N = \frac{n^2}{2\left(\frac{2\pi m^* kT}{h^2}\right)^{3/4} \exp\left(-\frac{\Delta E}{2kT}\right)} \tag{5}$$

The dielectric constant [5] ε is calculated by using the expression

$$\varepsilon^2 = \frac{13.53}{\Delta E} \cdot \frac{m^*}{m_0} \tag{6}$$

Thus the electrical properties of GaX, InX (X=As, P and Sb), $Al_xGa_{1-x}As$, $Ga_xIn_{1-x}Sb$ and Si_xGe_{1-x} can be calculated by using only two parameters lattice constant and activation energy.

3. Discussion and conclusions

The theoretical study has been made on binary III-V compounds on GaX, InX (X=As, P and Sb). And, the study has been extended to IV-IV compound Si_xGe_{1-x} and ternary compounds on $Al_xGa_{1-x}As$ and $Ga_xIn_{1-x}Sb$ as a function of composition x. Table 1 gives the values of lattice constant and activation energy used for the present study [1, 2, 8-10]. Table 2 gives the calculated values of the electrical properties such as carrier concentration (n), carrier mobility (u), carrier effective mass (m*), dielectric constant (ε) and electrical resistivity of GaX, InX (X=As, P and Sb). The values are compared with the reported experimental results in Fig. 1a and the same for $Al_xGa_{1-x}As$ [18] is shown in Fig 1b as a function of composition 'x'. The Fig. 2 shows the comparison of validation of theoretical and experimental electrical resistivity on $Ga_xIn_{1-x}Sb$ and Si_xGe_{1-x} [19] for various values of composition 'x'. They are found to be in good agreement with each other. The limitation of this study is that it can be applied only to semiconductors and not to metals because of the dependence of the activation energy on the energy gap. Therefore, the present study has been restricted only to the semiconductors and not to metals. However, the theoretical study gives a reasonably good description of electrical properties as a function of composition using only two parameters lattice constant and activation energy.

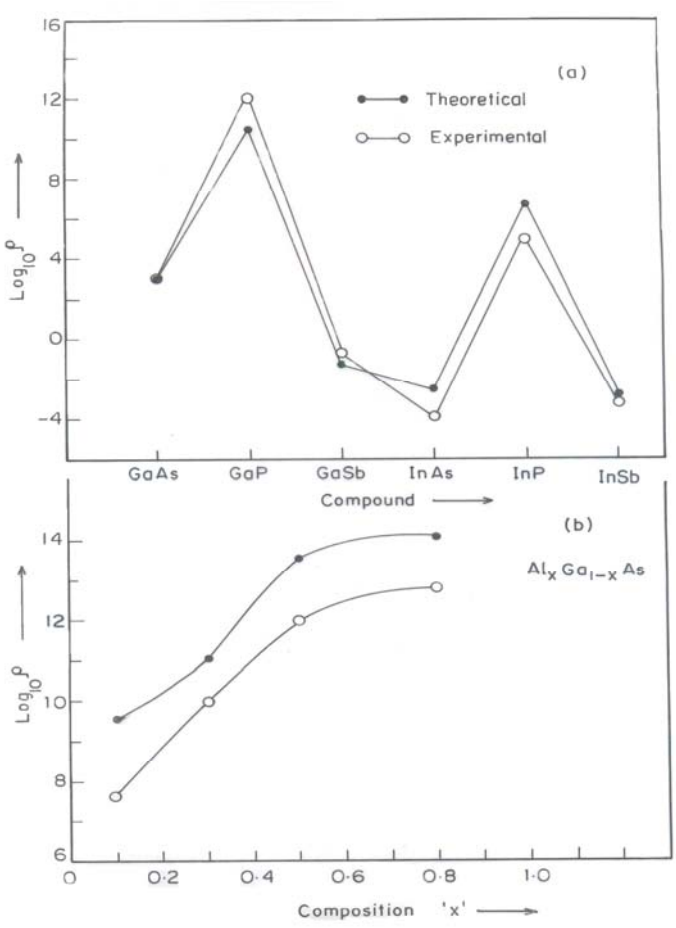

Fig.1. The plot of theoretical and experimental electrical resistivity of GaX, InX (X=As, P and Sb) and (b) $Al_xGa_{1-x}As$ as a function of composition "x".

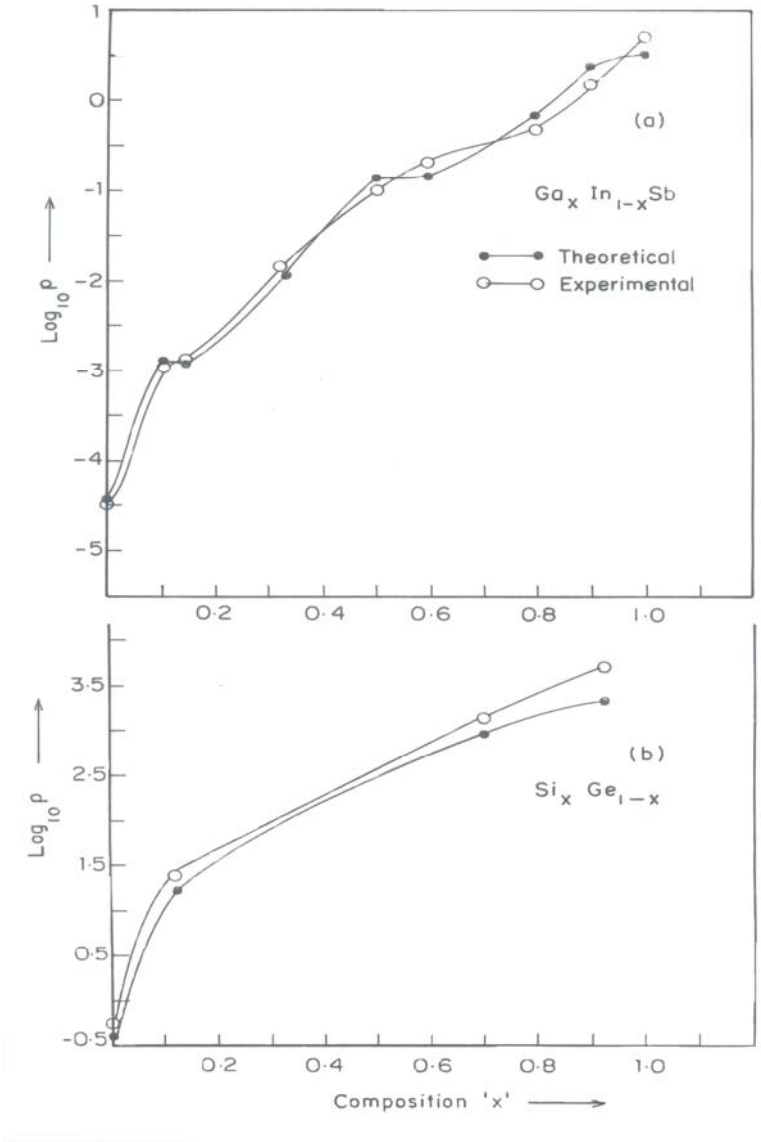

Fig.2. The plot of theoretical and experimental electrical resistivity of $Ga_xIn_{1-x}Sb$ and Si_xGe_{1-x} as a function of composition "x".

Table 1. The values of lattice constant (a in Å) and Activation energy (ΔEg in eV) used for the present study

Compound	x	a in Å	ΔEg in eV	Ref
GaAs	-	5.650	1.420	[1]
GaP	-	5.451	2.261	[2]
GaSb	-	6.095	0.720	[2]
InAs	-	6.058	0.350	[2]
InP	-	5.869	1.351	[2]
InSb	-	6.479	0.180	[2]
$Al_xGa_{1-x}As$	0.10	5.654	1.549	[8]
	0.30	5.656	1.798	[8]
	0.50	5.657	1.998	[8]
	0.80	5.660	2.092	[8]
$Ga_xIn_{1-x}Sb$	0.00	6.495	0.172	[9]
	0.10	6.450	0.190	[9]
	0.14	6.430	0.199	[9]
	0.32	6.360	0.259	[9]
	0.50	6.300	0.345	[9]
	0.59	6.250	0.405	[9]
	0.79	6.180	0.549	[9]
	0.90	6.140	0.633	[9]
	1.00	6.100	0.726	[9]
Si_xGe_{1-x}	0.00	5.660	0.650	[10]
	0.12	5.630	0.800	[10]
	0.68	5.485	0.940	[10]
	0.92	5.435	1.300	[10]

Table 2. The Calculated values of the carrier concentration (n), carrier.

Compound	x	n	m^*x10^{31}	ε	u $m^2V^{-1}Sec^{-1}$
GaAS	-	$1.923\ x10^{13}$	6.819	2.671	$3.150x10^{2}$
GaP	-	$1.888\ x\ 10^{6}$	7.426	2.209	$1.280x10^{2}$
GaSb	-	$1.144\ x\ 10^{19}$	5.805	3.461	$1.071x10^{1}$
InAs	-	$8.918x10^{21}$	4.168	4.206	$1.253x10^{-2}$
InP	-	$7.375x10^{13}$	6.863	2.747	$1.506x10^{-2}$
InSb	-	$1.474x10^{23}$	3.021	4.993	$4.495x10^{-2}$
$Al_xGa_{1-x}As$	0.10	$1.648x10^{23}$	6.967	2.585	$9.590x10^{-4}$
	0.30	$1.393x10^{10}$	7.202	2.460	$4.241x10^{-3}$
	0.50	$2.998x10^{8}$	7.357	2.339	$5.639x10^{-4}$
	0.80	$5.002x10^{7}$	7.422	2.296	$9.849x10^{-4}$
$Ga_xIn_{1-x}Sb$	0.00	$1.652x10^{23}$	2.940	5.039	1.138
	0.10	$1.270x10^{23}$	3.113	4.933	$3.706x10^{-2}$
	0.14	$1.101x10^{23}$	3.202	4.881	$5.071x10^{-2}$
	0.32	$4.359x10^{22}$	3.713	4.615	$1.126x10^{-2}$
	0.50	$1.030x10^{22}$	4.315	4.308	$4.664x10^{-3}$
	0.59	$3.630x10^{21}$	4.641	4.126	$1.234x10^{-2}$
	0.79	$2.717x10^{20}$	5.276	3.779	$3.906x10^{-2}$
	0.90	$5.743x10^{19}$	5.562	3.612	$4.461x10^{-2}$
	1.00	$1.024x10^{19}$	5.826	3.452	$1.183x10^{-1}$
Si_xGe_{1-x}	0.00	$3.822x10^{19}$	5.262	3.468	$4.667x10^{-1}$
	0.12	$2.363x10^{18}$	5.692	3.230	$1.760x10^{-1}$
	0.68	$1.673x10^{17}$	5.921	3.059	$4.150x10^{-2}$
	0.92	$1.832x10^{14}$	6.523	2.730	$1.879x10^{1}$

Mobility (u), carrier effective mass (m*), dielectric constant (ε)

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