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Theoretical Study of Electrical Properties of a Germanium and Gallium Arsenide P-N Junction Diode in an Open Circuit

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Abstract

Theoretical study of electrical properties of a Germanium and Gallium arsenide p-n junction diode in an open circuit is investigated using one dimensional Poisson equation. It is assumed that the conduction electrons and holes obey Boltzmann equation of statistical mechanics. The comparison of electrical properties variation within the p-n junction for the two semi-conductor materials is describe and discussed. There is high intrinsic concentration in elemental semiconductor Ge, while the bond existing in doped semiconductor $GaAs$ results in lesser value. The corresponding electron and hole concentrations, the temperature values are within (200 – 500) K. The curves for a plane p-n junction in germanium and gallium arsenide are presented in figures 2 and 3.

Keywords: Elemental Semiconductor; Electrical Properties; Intrinsic Concentration; Electron Concentration; Hole Concentration

INTRODUCTION

Semiconductors are groups of materials having electrical conductivities intermediate between metals and insulators. It is significant that the conductivity of these materials can be varied over orders of magnitude by changes in temperature, optical excitation, and impurity content. The variability of electrical properties makes the semiconductor materials natural choices for electronics device investigations (Ben, 1995). Semiconductor materials are found in column IV and neighboring columns of the periodic table (Table 1-1). The column IV semiconductors, silicon and germanium, are called elemental semiconductors because they are composed of single species of toms (Ben, 1995). In addition to the elemental materials, compounds of column III and V atoms, as well as certain combination from II and VI, make up intermetallic, or compound, semiconductors. Resolving electron and hole transport properties in semiconductor materials by constant light-induced magneto transport Artem et al., (2024).

Table 1: Common semiconductor materials: (a) the portion of the periodic table where semiconductors occur; (b) elemental and compound semiconductor

(a)	II	III	IV	V	VI
		B	C		
		Al	Si	P	S
	Zn	Ga	Ge	As	Se
	Cd	In	Sb	Te	

(b) Elemental	IV Compounds	Binary III-IV Compounds	Binary II-VI Compounds
Si	SiC	AIP	ZnS
Ge	SiGe	AIAs	ZnSe
		AISb	ZnTe
		GaP	CdS
		GaAs	CdSe
		GaSb	CdTe
		InP	
		InAs	
		InSb	

The elemental semiconductor Ge was widely used in the early days of semiconductor development for transistors and diodes. Si is now used for the majority of rectifiers, transistors and integrated circuits. Crisp et al., (2004) predict the electrical power output by Gallium Arsenide/ Germanium solar cells at the surface of Mars. Trevor and Xiaofeng, (2016) stated that pure germanium element can be doped with arsenic or other elements and used as a transistor in electronic applications. However, the compounds are widely used in high-speed devices requiring the emission or absorption of light. The two-element (binary) III-V compounds such as GaAs and GaP are common in light-emitting diode (LEDs) (Ben, 1995). Three-element (ternary) compounds such as GaAsP and four-element (quaternary) compounds such as InGaAsP can be grown to provide added flexibility in choosing materials properties. Si and Ge are also widely used as infrared and nuclear radiation detectors. The 500 nm process which is a common process for GaAs makes it difficult to build integrated circuits that has small structures because of its high impurity density Schlesinger, (2001*)*. GaAs wafers are used in laser diodes, photodetectors, and radio frequency (RF) amplifiers for mobile phones and base stations Green, (2024). GaAs transistors are also essential to monolithic microwave integrated circuits (MMICs), used in satellite communication and radar systems, as well as in low-noise amplifiers (LNAs) that enhance weak signals (Ishutkin and Kagadey, 2015*)*.

Electron and Holes

In semiconductor, mobility of free electrons and holes bands with reasonably energy gap is an important measured quality Maksym et al., (2023). Donor and acceptor atoms are atoms of foreign substances that added in minute amounts (approximately one part per million) to the basic semiconductor material, which is usually germanium or silicon. Since they are fixed in the crystal lattice, they constitute fixed charges. Geoffrey, (2021) The electron-hole has absolute values of the same charge, but unlike the electron, it is positive. The additions of donor atoms add conductor electrons without addition corresponding holes yields n-type material, which conducts mostly by negatively charge electrons. Similarly, the addition of acceptor atom gives p-type material which conducts mostly by positively charge holes.

Intrinsic Material and Extrinsic Material

A perfect semiconductor crystal with no impurities or lattice defects is called an intrinsic semiconductor. In such material there are no charge carriers at $0\ K$, since the valence band is filled with electrons and the conduction band is empty. At higher temperatures, electron-hole pairs are generated as valence band electrons are excited thermally across the band gap to the conduction band. These electron-hole pairs (EHPs) are the only charge carriers in intrinsic materials (Ben, 1995). Each of these intrinsic carrier concentrations is commonly referred to as ni. Thus for intrinsic material,

$$n = p = ni \tag{1}$$

In addition to the intrinsic carrier generated thermally, it is possible to create carriers in semiconductors by purposely introducing impurities into the crystal by doping, which is the most common technique for varying the conductivity of semiconductors (Ben, 1995). By doping, a crystal can be altered so that it has a predominance of either electron or holes, when a crystal is doped such that the equilibrium carrier concentrations no and po are different from the intrinsic carrier concentration ni, the material is said to be extrinsic.

Junction Diodes

Most semiconductor devices contain at least one junction between p-type and n-type material. These p-n junctions are fundamental to the performance of functions such as rectification, amplification, switching, and other operations in electronic circuits. A p-n junction may be formed from a single-crystal intrinsic semiconductor by doping part of it with impurities and the remainder with donors.

Theoretical background

Determinations of intrinsic concentrations

The effective density of states in the conductor band is given by the expression

$$N_C = 2\left(\frac{2\pi m_n{*}K_B T}{h^2}\right),$$

$$= 2\left(\frac{2\pi m_n{*}K_B T}{h^2}\right)^{3/2} T^{3/2} \tag{2}$$

The effective density of state in the valence band is given by the expression

$$N_V = 2\left(\frac{2\pi m_p * K_B T}{h^2}\right),$$

$$= 2\left(\frac{2\pi m_p * K_B T}{h^2}\right)^{3/2} T^{3/2} \tag{3}$$

The intrinsic electron and hole concentrations are equal (since the carriers are created in pairs), $n_i = p_i$; thus, the intrinsic concentration is given by the relation

$$n_i = \sqrt{N_C N_V} exp\left(-E_g/2K_B T\right) \tag{4}$$

Substituting equation (2) and (3) into (4), intrinsic concentrations become:

$$n_i(T) = 2\left(\frac{2\pi K_B T}{h^2}\right)^{3/2} \left(m_n * m_p\right)^{3/4} exp\left(-E_g/2K_B T\right),$$

$$= 2\left(\frac{2\pi K_B T}{h^2}\right)^{3/2} T^{3/2} \left(m_n * m_p\right)^{3/4} exp\left(-E_g/2K_B T\right) \tag{5}$$

where the expression is valid for either hole or electron. The intrinsic concentration is independent on both $T^{3/2}$ and $exp(1/T)$, the exponential temperature dependence dominates $n_i(T)$, where we have plotted $\ln n_i\ (T) vs\ 1000/T$, it appears linear.

Table 2. Effective mass values for Si, Si and $GaAs$. The free electron rest mass is m_o.

	Ge	Si	$GaAs$
$m_n{}^*$	0.55 m_o	1.1 m_o	0.067 m_o
$m_p{}^*$	0.37 m_o	0.56 m_o	0.48 m_o

Electron and hole Concentrations

The Fermi distribution function can be used to calculate the concentrations of electrons and holes in a semiconductor, if the densities of available states in the valence and conduction bands are known. For example, the concentration of electrons in the conduction band is given by the equation.

$$n_o = \int_{EC}^{\infty} f(E) N(E) dE,$$

Where $N(E)dE$ is the density of states (cm^3) in the energy range dE. The subscript O used with the electron and hole concentration symbols (N_O, P_o) indicator equilibrium conditions.

The number of electrons per unit volume in the energy range dE is the product of the densities of states and the probability of occupation $f(E)$. Thus the total electron concentration is the integral over the entire conduction band. The function $N(E)$ can be calculated by using quantum mechanics and the Pauli Exclusion Principle.

If we count the electron states per energy level in accordance with the Pauli principle, the number of states with energy level less than n is twice the volume in n-space, $2(2\pi/3)n^2$. Thus the total number of states in the volume V can be expressed as

$$NV = \frac{8\pi}{3}n^3 \tag{6}$$

The energy of the nth energy level is $E_n = \frac{h^2n^2}{2mV^{2/3}}$,

$$= \frac{h^2n^2}{2mV^{2/3}}\left(\frac{NV}{8\pi/3}\right)^{2/3},$$

$$= \frac{h^2}{2m}(3\pi^2N)^{2/3} \tag{7}$$

The total number of states per volume is

$$N\int N(E)dE = \frac{1}{3\pi^2}\left(\frac{2mE}{h^2}\right)^{3/2} \tag{8}$$

Differentiating equation (8), we obtain

$$N(E) = \frac{1}{3\pi^2}\left(\frac{3}{2}\right)\left(\frac{2m}{h^2}\right)^{3/2}E^{1/2},$$

$$= \frac{1}{2\pi^2}\left(\frac{2m}{h^2}\right)^{3/2}E^{1/2} \tag{9}$$

The probability of occupancy f any energy level E is

$$F(E) = \frac{1}{e^{\left(E-E_f\right)/K_BT+1}} \tag{10}$$

The density of occupied electron states Ne in dE is

$$N_e dE = N(E)f(E)dE \tag{11}$$

We may calculate the concentration of electrons in the conduction band at a given temperature by integrating equation (11) across the band;

$$n = \int_0^\infty N(E)f(E)dE,$$

$$= \frac{1}{2\pi^2}\left(\frac{2m}{h^2}\right)^{3/2} e^{E_f/K_BT} \int_0^\infty E^{1/2} e^{-E_g/K_BT} dE \tag{12}$$

The integral in equation (12) is of the standard form;

$$\int_0^\infty X^{1/2} e^{-ax} dx = \frac{\sqrt{\pi}}{2a\sqrt{a}} \tag{13}$$

Thus equation (12) gives

$$n = 2\left(\frac{2\pi K_BT}{h^2}\right)^{1/2} exp\left(E_f/K_BT\right) \tag{14}$$

If we refer to the bottom of the conduction band as Ec, instead of $E = 0$, the expression for the electron concentration is

$$n = 2\left(\frac{2\pi K_BT}{h^2}\right)^{1/2} exp\left(E_f - E_c/K_BT\right) \tag{15}$$

Under normal condition the electron and hole satisfy the Boltzmann equation of statistical mechanics:

$$p = p_i exp\left(-E_g/K_BT\right), \tag{16}$$

$$n = n_i exp\left(E_g/K_BT\right) \tag{17}$$

Since the temperature is varied, the value of n_i obtained in equation (4) is substituted into equations (17 and (18) to obtain the corresponding electron and hole concentrations, the temperature values are within (200 – 500) K. Curves for a plane p-n junction in germanium and gallium between (200 – 500) K are shown in figures (2) and (3).

Electric Field and Electric Potential at Room Temperature

To calculate the electric field distribution within the transition region, we begin with Poisson's equation, which relates the gradient of the electric field to the local space charge at any given point X:

$$\frac{dE(x)}{dx} = \frac{q}{\varepsilon}(p - n + P - N) \tag{18}$$

where ε is the permittivity of the semiconductor. The space charge ρ is given by

$$\rho = q(p - n + P - N) \tag{19}$$

where q is the elementary electron charge , p is the mobile hole density, n is the mobile electron density. P and N are fixed hole and electron densities.

Combining equations (16), (17) and (18), the differential equation for E becomes;

$$\frac{dE(x)}{dx} = \frac{q}{\varepsilon}[(P - N)2n_o sinh(E_g/k_BT)],$$

$$(2n_o sinh(E_g/k_BT) - \left(\frac{2qP_0}{\varepsilon}\right)x \qquad (20)$$

where p_o and n_o are hole and electron concentration at room temperature.

Integrating equation (20), we obtain

$$E(x) = 2n_o \frac{q}{\varepsilon} sinh(E_g/k_BT)x - \frac{q}{\varepsilon} p_o x^2, \qquad (21)$$

If the term $\frac{q}{\varepsilon} p_o x^2$ is neglected since the value is infinitesimal and has no effect, the term with electron concentration dominates; thus

$$E(x) = 2n_o \frac{q}{\varepsilon} sinh(E_g/k_BT)x$$

Electric field variation within the depletion region is depicted in figure (3.4) and (3.5). The expression for electric potential is obtained by integrating equation (21). It is given by

$$V(x) \approx -n_o sinh\left(E_g/k_BT\right)x^2 \qquad (22)$$

The curves of $V(x)$ versus distance are shown in figure (4) and (5).

The electric charge density at room temperature

The Poisson's equation which has been described in equation (18) is used, recall that;

$$\frac{dE(x)}{dx} = \frac{\rho}{\varepsilon},$$

$$\rho = \varepsilon \frac{dE(x)}{dx} \qquad (23)$$

Substituting equation (20), thus;

$$p(x) = 2n_o q sinh(E_g/k_BT) - 2qp_o x,$$

The term $2qp_o x$, is very small thus;

$$p(x) = 2n_o q sinh(E_g/k_BT) \qquad (24)$$

The relationship between electric charge density and distance is plotted in figure (6) and (7).

RESULTS

Table 3. Computed values of intrinsic concentrations

$T\ (K)$	$1000/T\ (K-1)$	Ge		$GaAS$	
		$ni\ (T)$ (cm^{-3})	$ln\ ni\ (T)$ (cm^{-3})	$ni\ (T)$ (cm^{-3})	$ln\ ni\ (T)$ (cm^{-3})
200.00	5.00	1.52 x 10^{16}	37.26	1.03 x 10^{6}	13.85
250.00	4.00	1.03 x 10^{18}	41.48	5.57 x 10^{9}	22.47
300.00	3.33	1.81 x 10^{19}	44.34	1.90 x 10^{12}	28.27
350.00	2.86	1.45 x 10^{20}	46.42	1.24 x 10^{14}	32.45
400.00	2.50	7.08 x 10^{20}	48.01	2.92 x 10^{15}	35.61
450.00	2.22	2.49 x 10^{21}	49.27	3.49 x 10^{16}	38.09
500.00	2.00	6.90 x 10^{21}	50.29	2.58 x 10^{17}	40.09

Table 4. Calculated values of hole concentrations

$T\ (T)$	$1000/T\ (K-1)$	Ge		$GaAS$	
		$P(cm^{-3})$	$ln\ P(cm^{-3})$	$P\ (cm^{-3})$	$ln\ P\ (c$
200.00	5.00	0.21 x 10^{0}	-1.56	1.02 x 10^{-30}	-69.06
250.00	4.00	3.30 x 10^{4}	10.40	9.07 x 10^{9}	-43.85
300.00	3.33	1.03 x 10^{8}	18.45	1.89 x 10^{-12}	-26.99
350.00	2.86	3.33 x 10^{10}	24.23	3.32 x 10^{-7}	-14.92
400.00	2.50	2.16 x 10^{12}	28.58	2.91 x 10^{-3}	-5.84
450.00	2.22	3.93 x 10^{13}	32.00	3.48 x 10^{0}	1.25
500.00	2.00	1.23 x 10^{15}	34.75	1.02 x 10^{3}	6.93

Table 5. Computed values of electron concentrations

$T\ (K)$	$1000/T\ (K-1)$	Ge		$GaAS$	
		$n(cm^{-1})$	$ln\, n(cm^{-3})$	$n\ (cm^{-3})$	$ln\, n\ (cm$
200.00	5.00	1.12×10^{33}	76.10	1.04×10^{42}	96.75
250.00	4.00	3.22×10^{31}	75.55	3.64×10^{38}	88.79
300.00	3.33	3.19×10^{30}	70.24	1.91×10^{36}	83.54
350.00	2.86	6.31×10^{29}	68.62	4.64×10^{34}	79.82
400.00	2.50	1.92×10^{29}	67.43	2.93×10^{33}	77.06
450.00	2.22	7.82×10^{28}	66.53	3.50×10^{32}	74.94
500.00	2.00	3.86×10^{28}	65.82	6.49×10^{31}	73.25

Table 6. Calculated values of electric field and electric Potential

$x \times 10^{-2}(cm)$	Ge		$GaAs$	
	$x \times 10^{32}\ (v/cm)$	$v \times 10^{30}\ (v/cm^2)$	$E \times 10^{51}\ (v/cm)$	$V \times 10^{49}\ (v/cm^2)$
-1.0	-6.34	-3.17	-2.63	-1.31
-0.8	-5.04	-2.03	-2.10	-0.84
-0.6	-3.81	-1.14	-1.58	-0.47
-0.4	-2.54	-0.51	-1.05	-0.21
-0.2	-1.27	-0.13	-0.53	-0.05
0.2	1.27	-0.13	-0.53	-0.05
0.4	2.54	-0.51	-1.05	-0.21
0.6	3.81	-1.14	-1.58	-0.47
0.8	5.04	-2.03	-2.10	-0.84
1.0	6.34	-3.17	-2.63	-0.31

Table 7. Computed values of electric charge density

$x \times 10^{-2}$ (cm)	Ge	$GaAs$
	$\rho \times 10^{22}$	$\rho \times 10^{41}$
-1.0	8.98	3.07
-0.8	8.98	3.07
-0.6	8.98	3.07
-0.4	8.98	3.07
-0.2	8.98	3.07
0.2	8.98	3.07
0.4	8.98	3.07
0.6	8.98	3.07
0.8	8.98	3.07
1.0	8.98	3.07

DISCUSSION

Two semiconductor materials were compared and their respective electrical properties studied reveal that they exhibit similar characteristics in their behaviour with little differences occurring only in values obtained from each calculation carried out. The results obtained are shown in tables 3 – 7. The graph of $\ln ni(T)$ against 1000/T is a linear relationship as depicted in figure 1; it is observed that the intrinsic concentration increases as the temperature increases. The value obtained for Ge is higher than that of $GaAs$ because Ge is an elemental semiconductor and it is made up of single species of atom while $GaAs$ is an intermetallic semiconductor made up of mixed species of atoms. Figures 2 and 3 shows the curve of the variation of the carrier concentration with temperature, the hole concentration increases as the temperature increases with the value in Ge higher than that in $GaAs$, while the electron concentration decreases with an increase in temperature; the value in $GaAs$ is higher than that obtained in Ge at any given temperature. This shows that as the temperature increases, more holes diffuse from the p side to the n side of the material and conversely, few electrons diffuse from the n side to the p side of material. The plot of electric field against distance is a linear relationship as shown in figure 4, the values obtained in either graphs are higher because the electron concentration dominates while the effect of hole concentration is not noticeable. The electric field increase from the negative distance direction towards the positive distance direction, it goes to zero at the junction of the transition region. The parabolic curve of electric potential is revealed in figure 5, the values in $GaAs$ is higher than that obtained in Ge; the values are negative throughout the width of the depletion region. Since it is negative, it pints away from n-type material, which contains a majority of fixed positive charges.

Figures: 6 and 7 show the plot of electric charge density against distance. It is constant with the transition region. Electrons and holes are in transit from one side of the junction to the other. Some electrons diffuse from n to p, and some are swept by the electric field from p to n (and conversely from hole); there are however, very few carriers within the transition region at any given time, since electric field serves to sweep out carrier which have wandered into the depletion region.

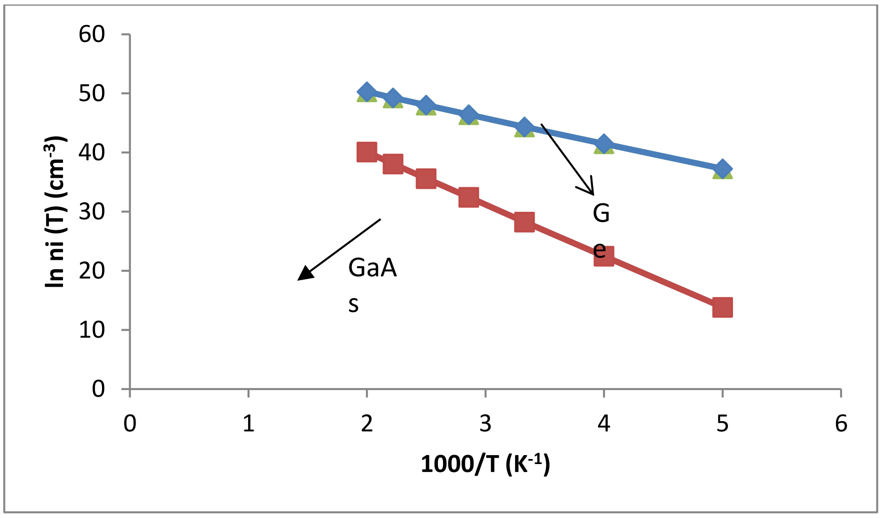

Figure 1: Graph of ln ni against 1000/T for Ge and GaAs

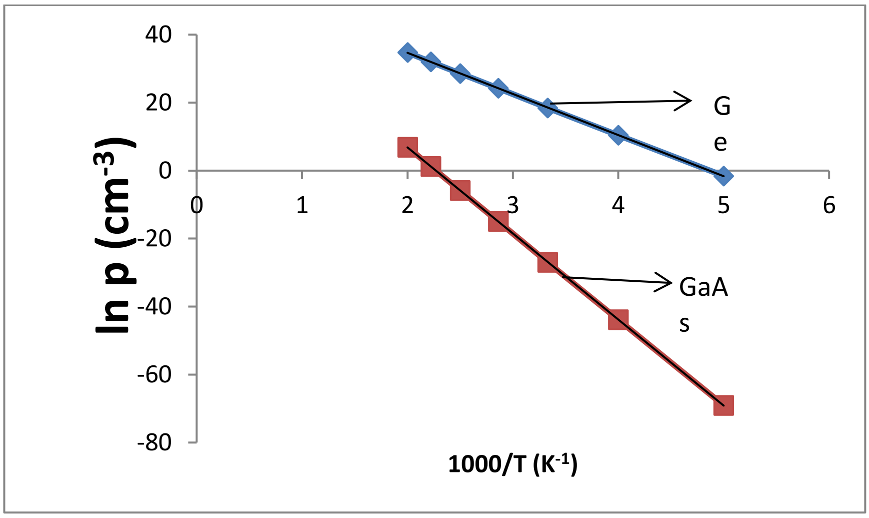

Figure 2: Graph of ln p against 1000/T for Ge and GaAs

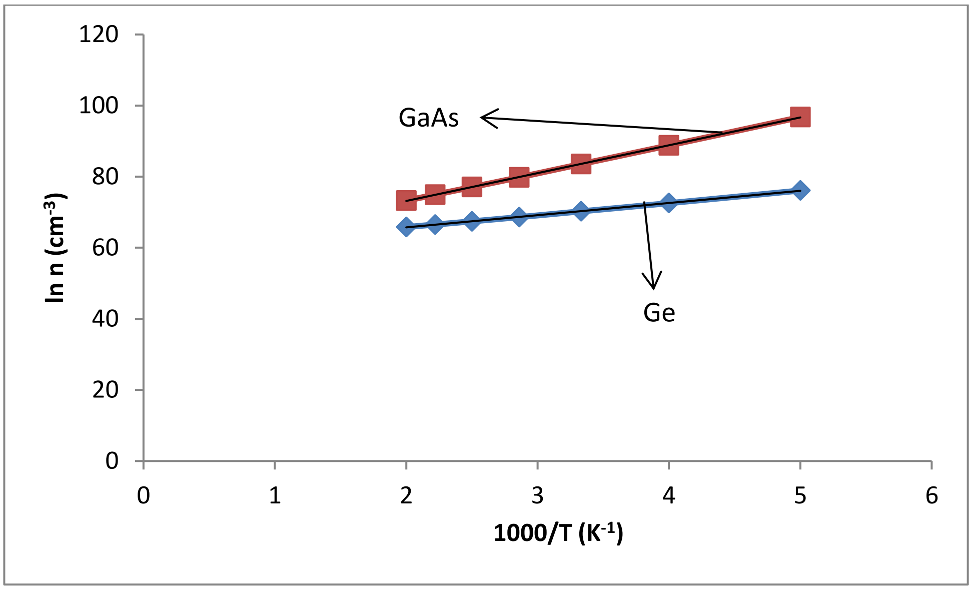

Figure 3: Graph of ln n(T) against 1000/T for Ge and GaAs

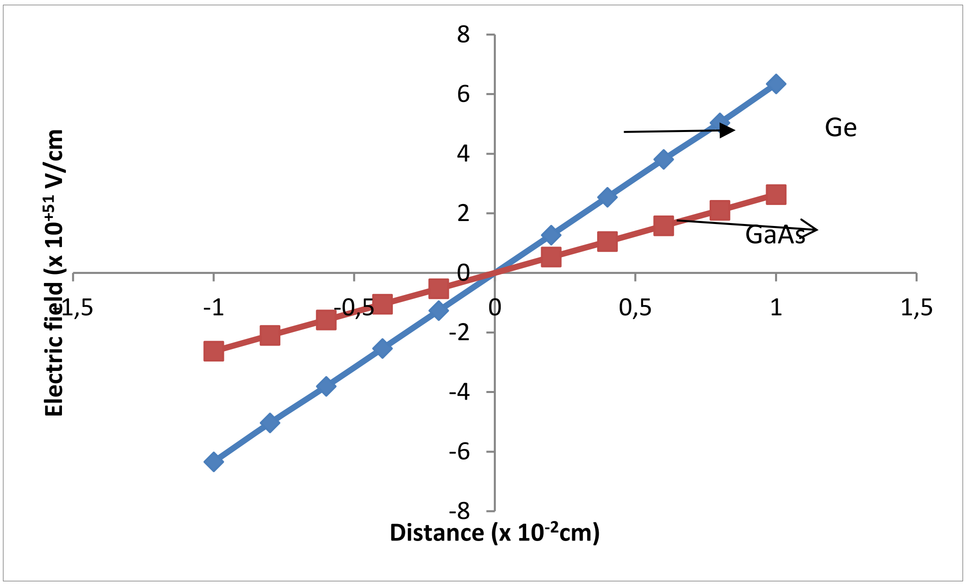

Figure 4: Graph of electric field against distance for Ge and GaAs.

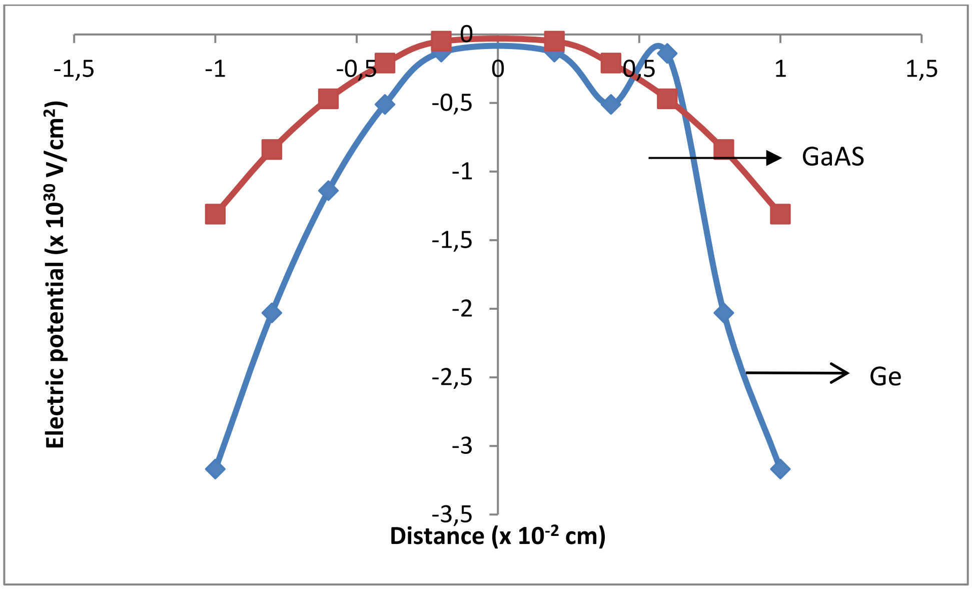

Figure 5: Graph of electric potential against distance for Ge and GaAs.

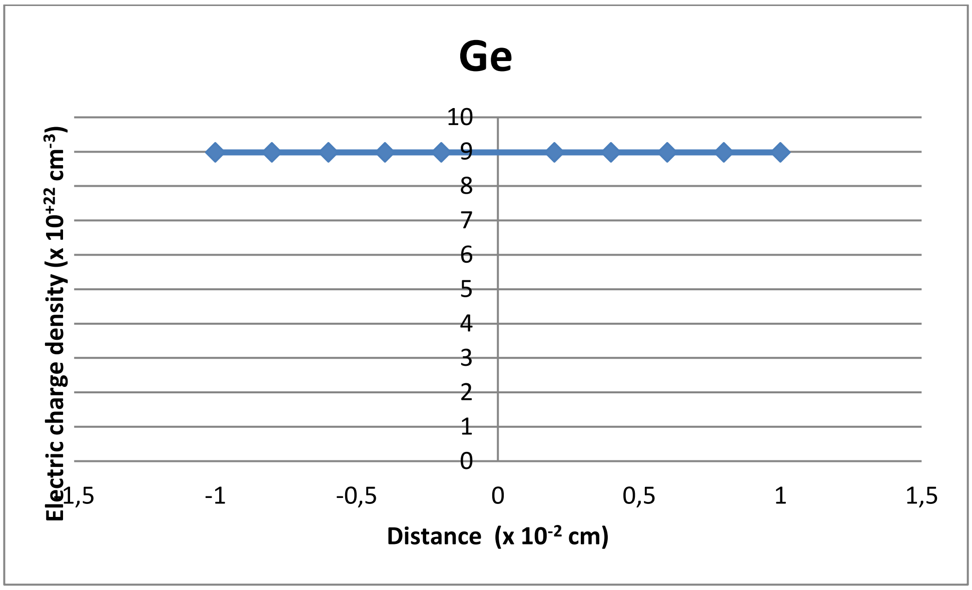

Figure 6: Graph of electric charge density against distance for Ge

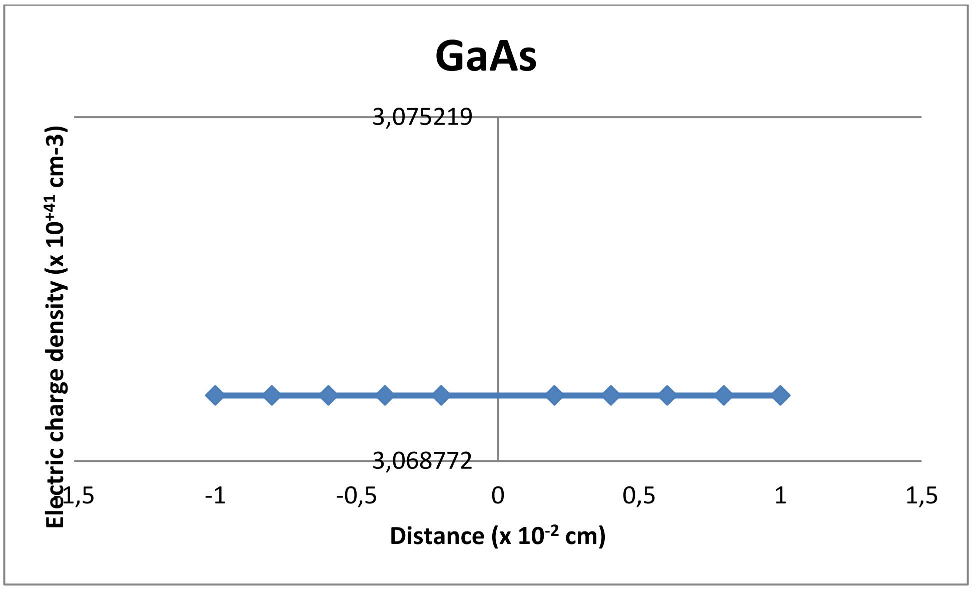

Figure 7: Graph of electric charge density against distance for GaAs

CONCLUSION

There is high intrinsic concentration in elemental semiconductor Ge, while the bond existing in doped semiconductor $GaAs$ results in lesser value. The hole and electron concentration value are almost linear, the mixed bonding in $GaAs$ in which both ionic and covalent bonding forces participate made the electron concentration to be more than the observed in Ge, the reverse is the case in hole concentration. The electric field in both Ge and $GaAs$ have similar properties. It is maximum at the edge of the transition region with the value obtained in Ge lower than the observed value in $GaAs$. The electrical potential and electric charge density are also similar but the value obtained in $GaAs$ are higher than the observed in Ge; this means that all the properties exhibit by $GaAs$ is peculiar of intermetallic semiconductor and Ge of elemental semiconductor.

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Appendix 1: List of Symbols

E_f	Equilibrium Fermi Level (J, eV)
Eg	Band gap energy (J, eV)
$f(E)$	Fermi-Dirac distribution function
h	Planck constant $(J - S, eV - s)$
$\hbar$	Planck's constant divided by 2π $(J - S, eV - s)$
K_B	Boltzmann's constant $(J/K, eV/K)$
m, m^*	Mass, effective mass (kg)
m_o^*, m_p^*	Effective mass for electrons, holes (kg)
m_o	Rest mass of the electron (Kg)
n	Concentration of electrons in the conduction band (cm^{-3})
n_i	Intrinsic concentration of electrons (cm^{-3})
n_o	Equilibrium concentration of electrons (cm^{-3})
N_a, N_d	Concentration of acceptors, donors (cm^{-3})
N_C, N_V	Effective density of states at the conduction band, valence band (cm^{-3})
P	Concentration of holes in the valence band (cm^{-3})
Pi	Intrinsic hole concentration $(cm^{-3}) = n_i$
P_o	Equilibrium hole concentration (cm^{-3})
q	Magnitude of electron charge (C)

$\varepsilon,\ \epsilon,\ \varepsilon_o$ Permittivity, relative dielectric constant & permittivity of free space; $(F/cm);\ \varepsilon = \varepsilon_r\varepsilon_o$

Appendix 2: Properties of Semiconductor Materials used

	$E_g(eV)$	ε_o
Ge	0.67	16
$GaAs$	1.43	13.2

Appendix 3: Physical Constanta and Conversion Factors

Boltzmann Constant	$k_B = 1.38 \times 10^{-23}\,J/K$
Electronic Charge (magnitude)	$q = 1.60 \times 10^{-19}C$
Electronic rest mass	$m_o = 9.11 \times 10^{-31}Kg$
Permittivity of free space	$\varepsilon_o = 8.85 \times 10^{-14}F/cm$
Planck's constant	$h = 6.63 \times 10^{-34}J - s$
$1\ eV = 1.60 \times\times 10 - 19\,J$	

Appendix 4

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C                 PROGRAM TO FIND THEHOLE AND ELECTRON CONCENTRATION IN Ge
C                 AT DIFFERENT VALUE OF TEMPERATURE, T(k)
                  DIMENSION Xni(20), P(20), Xn(20)
                  OPEN (1, FILE = 'ABI.OUT', STATUS = 'NEW')
                  J = 1
                  T = 200.0
                  WRITE (1, *)'                     Ge'
                  WRITE (1, *)' T  TS                P       Xn'
                  DO 10    I = 1, 7
                  Xni (1) = 1.52 E + 16
                  Xni (2) = 1.03 E + 18
                  Xni (3) = 1.81 E + 19
                  Xni (4) = 1.45 E + 20
                  Xni (5) = 7.08 E + 20
                  Xni (6) = 2.49 E + 21
```

```
                Xni (7) = 6.90 E + 21
                Xk = 1.38 E – 23
                Q = 1.6 E -23
                Eg = 0.67 * 2
                A = Eg/ (Xk * T)
                P (J) = Xni (j) * Exp (-A)
                Xn(J) = Xni (J) * Exp (A)
                TS = 1000.0/T
                WRITE (1, 8) T, TS, P(J), Xn(J)
8               FORMAT (3X, 2F 6.2, 2? (3X, E8.3)
                T = T) 50.0
                J = J = 1
10              CONTINUE
                STOP
                END
```