Gamma Irradiation Effects on n-ZnSe/n-Si Isotype Heterojunctions

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Abstract

To get an insight into the isotype heterojunction (IHJ) properties, the influence of gamma irradiation (GI) on the structural and electrical properties of n-ZnSe/n-Si has been presented. The ZnSe thin films were deposited onto the n-Si substrate by thermal evaporation technique. The X-ray diffraction (XRD) studies revealed the nanocrystalline nature of ZnSe thin films with prominent (111) orientation. The gamma irradiated samples displayed no crystallographic phase transformation up to 10 kGy irradiation doses. But noticeable and inconsistent modifications in the different lattice parameters were observed due to irradiation-induced effects. From the analysis of I-V characteristics, it has been found a similar trend in the variation of lattice mismatch, Schottky barrier height and interface trap parameter at different irradiation doses. Thus demonstrating the poor rectification properties of n-ZnSe/n-Si IHJs due to intrinsic and gamma-induced defects, and their role in the space charge limited conduction (SCLC) mechanism that significantly dominating over the thermionic emission (TE) mechanism across the barrier.

Keywords Isotype heterojunctions · Gamma irradiation · Schottky barrier height · Lattice mismatch · Space charge limited conduction

1 Introduction

When two different semiconductors of the same type (n – or p – type) are brought into close contact, the resulting heterostructure is usually referred to as n – n or p – p isotype heterojunction (IHJ). In p – n junctions, the currents are contributed from both electrons and holes, but in n – n and p – p IHJs, the currents are predominantly contributed from the electrons and holes respectively [1, 2]. Compared to p – n or Schottky junctions, the current-voltage (I – V) characteristics of IHJs are being fewer reported. In recent years, IHJs is slowly attracting the research community to the fundamental understanding of their properties. Particularly, silicon based IHJs with large lattice mismatch ( ), for example, $InGaN/Si$ (17%) [2], Ge/Si (4.2%) [3] and ZnO/Si (40.1%) [4], were being reported to gain insight into the IHJ properties as well as

their possible applications, despite experimental difficulties in accounting role of defects due to greater lattice mismatch. Generally, the p – p IHJs are not preferred for high-speed electronic applications due to large effective mass and less mobility of holes [2]. But n – n IHJs have applications in different optoelectronic devices such as solar cells and injection lasers [1], photodetectors [2, 5, 6] and light emitting diodes (LEDs) [7].

From the fundamental and technological point of view, the semiconductor thin film growth on Si substrate is attractive by considering the possibility of monolithic integration of grown thin film for different applications. Recently, for instance, ZnO/Si heterostructure LEDs have stirred up considerable interest in integrating ZnO onto Si technology [2, 4, 6, 7]. Among the zinc chalcogenide family, $ZnSe$ possess quite interesting properties, particularly, its direct wide bandgap (2.7 eV) and intrinsic n – type conductivity which offers several applications in the field of optoelectronics, such as blue LEDs and lasers [8], thin film solar cells [9], second harmonic generation [10] and nonlinear switching [11]. Despite considerable interest, very few reports are available on the electrical properties of $ZnSe$ based heterojunctions. In particular, understanding $ZnSe/Si$ heterojunctions are essential for integrating $ZnSe$ onto Si technology. In this view, the present study deals with the

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fundamental understanding of $n - \text{ZnSe}/n - \text{Si}$ IHJs by accounting junction $I - V$ characteristics. In addition, to have an insight into junction properties such as lattice mismatch, interface defects and Schottky barrier height, we have deliberately introduced defects by gamma irradiation. The consequent effects are outlined in the paper.

Usually, irradiation studies are carried out to account for the nature of intrinsic defects as well as irradiation-induced defects in the materials. However, the defects can be induced only if the incident radiation energy is greater than the displacement threshold energy (E_D) of constituting atoms in the material. The displacement threshold energies for Zn and Se atoms are about 10 and 8.2 eV respectively [12]. The electron, gamma, neutron and swift heavy ion irradiation are the most widely used techniques to introduce defects in the material. These irradiation studies are therefore not only useful in the fundamental understanding of the defect dynamics but also give insight into the material behaviour in the radiation environments. In the present study, prepared $n - \text{ZnSe}/n - \text{Si}$ IHJs have been subjected to $\text{Co} - 60$ gamma irradiation at different irradiation doses (up to 10 kGy) to account for irradiation induced modifications in the junction properties. Efforts were made to correlate the structural parameters with junction parameters and the underlying role of defects on the junction $I - V$ characteristics are presented in detail.

2 Materials and Methods

Phosphorus doped Si wafer ($n - \text{Si}$) having a doping concentration of $1.5 \times 10^{15} \text{ cm}^{-3}$ was procured from Sigma Aldrich, India. The wafer thickness was 500 μm , diced into dimensions of $0.5 \times 0.5 \text{ cm}$ and cleaned according to the standard procedures [13]. The high purity ZnSe compound of 99.999% was then deposited onto cleaned and diced $n - \text{Si}$ by thermal evaporation technique. The deposition was carried out at the rate of 2 $\text{\AA}/\text{s}$. A base pressure of $8 \times 10^{-6} \text{ mbar}$ was maintained during deposition. The thickness of the ZnSe thin film was kept at 100 nm by monitoring the quartz crystal [14].

The prepared $n - \text{ZnSe}/n - \text{Si}$ heterojunctions were subjected to gamma irradiation (GI) using $\text{Co} - 60$ source at Centre for Applications for Radioisotope and Radiation Technology (CARRT), Mangalore University, India. The $\text{Co} - 60$ source emits the photons of two energies, 1.17 and 1.33 MeV, which is well above the displacement threshold energies of ZnSe [12]. The dose rate of the $\text{Co} - 60$ gamma source during irradiation was 2.6 kGy/hr. The samples were exposed to the different GI doses in the range of 2 – 10 kGy (2, 4, 6, 8 and 10). The X-ray diffraction (XRD) studies were carried out using Rigaku Miniflex-600 diffractometer ($\text{Cu} - K\alpha$: 0.15402 nm). The junction $I - V$ characteristics were taken using Keithley source meter 2450 at room temperature and

under dark conditions. The aluminum pressure contacts were used as ohmic contacts during the measurements.

3 Results and Discussion

3.1 XRD Analysis

Figure 1 shows the XRD pattern of ZnSe thin film deposited on $n - \text{Si}$ substrate before and after GI. The peak at about 27° (2θ -value) is attributed to reflection from (111) plane of cubic phase ZnSe . This result is consistent with various reports of thermally evaporated ZnSe thin films having prominent (111) orientations [14–20]. No peaks from the hexagonal phase of ZnSe were noticed in the present study before and after GI, suggesting no crystallographic phase transformations. The lattice parameter of ZnSe has been evaluated from the prominent (111) peak by using the following simplified expression,

$$a_{\text{ZnSe}} = \frac{\sqrt{3}}{2} \frac{\lambda}{\sin \theta} \quad (1)$$

On the other hand, the XRD peak noticed at 69.2° (2θ -value) has been attributed to the prominent (400) reflection from $n - \text{Si}$ substrate. This peak is also consistent with various reports [13]. The lattice parameter of $n - \text{Si}$ is evaluated by using the following simplified expression [13],

$$a_{\text{Si}} = \frac{2\lambda}{\sin \theta} \quad (2)$$

where θ is Bragg's angle and $\lambda = 0.15402 \text{ nm}$ (wavelength of $\text{Cu} - K\alpha$). The other important deposited ZnSe thin film parameters such as crystallite size (D), lattice strain (ϵ), dislocation density (δ) and lattice mismatch (Δ) [21] were calculated by using the following relations [14–20]:

$$D = \frac{0.94\lambda}{\beta \cos \theta} \quad (3)$$

$$\epsilon = \left[\frac{\lambda}{D \cos \theta} - \beta \right] \times \frac{1}{\tan \theta} \quad (4)$$

$$\delta = \frac{15\epsilon}{aD} \quad (5)$$

$$\Delta = \frac{a_{\text{ZnSe}} - a_{\text{Si}}}{a_{\text{ZnSe}}} \quad (6)$$

where β is the full width at half maximum in radians. The evaluated values from Eqs. (1–6) are reported in Table 1.

In the present study, the a value of ZnSe deposited on $n - \text{Si}$ substrate was found to be 0.5693 nm. But lesser values have been reported for ZnSe thin films deposited on glass substrates (0.563 nm [15] 0.5637 nm [20]), and $p - \text{Si}$ substrate (0.5681 nm [17]). These results suggest that ZnSe deposited on $n - \text{Si}$ substrate has comparatively a greater value of a . Also, these

Fig. 1 (111) reflection of ZnSe thin films on n – Si substrate before and after gamma irradiation

marginal variations in a of ZnSe suggesting the role of n – Si substrate in increasing D and reducing ϵ and δ of the deposited thin film. ZnSe deposited on the glass substrate have D , ϵ and δ values of 19nm , 2.057×10^{-3} and $2.912 \times 10^{15}\text{m}^{-2}$ [20] respectively. While for ZnSe deposited on p – Si substrate have a , D , ϵ and δ values of 0.5681nm , 40.71nm , 9.5×10^{-4} and $6.03 \times 10^{15}\text{m}^{-2}$ respectively [17]. The latter values are similar to the present study (Table 1). However, an order of lesser values of δ in the present study suggests better quality of ZnSe thin films deposited the on n – Si substrate.

As noticed from Fig. 1, the gamma irradiated samples have exhibited no uniformity in the trend of (111) peak of ZnSe with the increase of GI dose. However, from Fig. 2, one can notice an inverse trade-off between D and ϵ as a function of GI dose. A similar trend has been also observed between D and δ , as the variation of ϵ and δ are similar because of Eqs. (4) and (5) respectively. However, no such trend has been noticed for variation in a of ZnSe for an increase in GI dose. These observations suggesting the complex nature of GI induced structural modifications in the n – ZnSe/ n – Si heterojunction properties. A similar inconsistent variation in a has been also reported for gamma irradiated Al/ n – Si Schottky junctions [13].

Table 1 Lattice parameters of Zn Se thin film deposited on n – Si substrate before and after gamma irradiation

Sample	a (nm) [ZnSe]	D (nm)	$\epsilon \times 10^{-4}$	$\delta \times 10^{14} \text{m}^{-2}$	a (nm) [Si]	Δ (%)
Unirradiated	0.5693	59.6	6.56	2.89	0.5426	4.69
2 kGy	0.5652	41.7	9.25	5.89	0.5426	3.99
4 kGy	0.5656	71.5	5.47	2.02	0.5426	4.06
6 kGy	0.5596	52.3	7.39	3.79	0.5425	3.06
8 kGy	0.5710	29.1	13.61	12.28	0.5426	4.97
10 kGy	0.5648	53.9	7.29	3.53	0.5423	3.98

3.2 Analysis of $I - V$ Characteristics by Thermionic Emission Theory

Figure 3 shows the $I - V$ characteristics of $n - \text{ZnSe}/n - \text{Si}$ IHJs before and after gamma irradiation. One can notice rectifying (Schottky) nature of the heterojunctions rather than ohmic type. However, the rectification ratios (rectification ratio, $RR = \text{forward current}/\text{reverse current}$) are small compared to that of Schottky or pn diodes. The rectifying nature suggests that there exists a potential barrier that must be overcome by the charge carriers (electrons) across the $n - n$ heterojunction. As Zn is metal and Se is metalloid, and the $I - V$ characteristics are mainly governed by electrons, the $n - n$ heterojunction properties in the present study can be accounted by applying thermionic emission (TE) theory of Schottky junctions.

According to TE theory, the forward current I across the junction for the applied voltage V is given by [22],

$$I = I_s \exp\left(\frac{qV}{\eta kT}\right) \left\{ 1 - \exp\left(-\frac{qV}{kT}\right) \right\} \quad (7)$$

where,

$$I_s = AA^{**} T^2 \exp\left(-\frac{q\Phi_{B0}}{kT}\right) \quad (8)$$

known as reverse saturation current, q is electronic charge, k is Boltzmann constant, T is absolute temperature, η is ideality factor, A is device area ($\sim 0.25 \text{ cm}^2$), A^{**} is Richardson constant (for $n - \text{Si}$, $A^{**} = 112 \text{ A} \cdot \text{cm}^{-2} \text{ K}^{-2}$ [13, 22]) and Φ_{B0} is zero-bias Schottky barrier height.

From Eq. (7), it follows that the plot of $\ln(I/\{1 - \exp(-qV/kT)\})$ against V gives a straight line even for values of V [22]. Thus, from the intercept and slope of the plot, one can determine Φ_{B0} and η respectively by using the following relations:

Fig. 2 Variation of particle size (D) and lattice strain (ϵ) of ZnSe deposited on $n - \text{Si}$ substrate before and after gamma irradiation

Fig. 3 $I - V$ characteristics of $n - \text{ZnSe}/n - \text{Si}$ IHJs before and after gamma irradiation

$$\Phi_{B0} = \frac{kT}{q} \ln \left[\frac{AA^{**} T^2}{I_s} \right] \quad (9)$$

and

$$\eta = \frac{q}{kT} \frac{dV}{d \ln(I/\{1 - \exp(-qV/kT)\})} \quad (10)$$

The straight line fits of the plots of $\ln(I/\{1 - \exp(-qV/kT)\})$ vs. V at lower voltage regions are given in Fig. 4 and the obtained values of Φ_{B0} and η from these plots are reported in Table 2.

However, Φ_{B0} and η values obtained from the TE theory (Eq. (7)) sometimes leads to an erroneous determination due to non-consideration of series resistance (R_s) in the evaluation procedure. The R_s is mainly presented from the heterojunction structure (bulk and interface) and ohmic contact regions. Therefore, by considering the effect of R_s in the evaluation procedure, one can obtain more reliable values of Φ_{B0} and η . In literature there exist different approaches to evaluate Φ_{B0} and η after the consideration of R_s in Eq. (7). In the present study, we applied the graphical method proposed by Cheung and Cheung, also known as the Cheung model [23]. The brief outline of the evaluation procedure is as follows:

The TE model Eq. (7), for the applied voltage $V > 3kT/q$ takes the form as:

$$I = I_s \exp \left[\frac{q(V - IR_s)}{\eta kT} \right] \quad (11)$$

The differentiation of Eq. (11) for I gives the relation,

$$\frac{dV}{d(\ln I)} = R_s I + \frac{\eta kT}{q} \quad (12)$$

Fig. 4 $\ln(I/[1 - \exp(-qV/kT)])$ vs. V plots of $n - \text{ZnSe}/n - \text{Si}$ IHJs before and after gamma irradiation

Therefore, the slope and intercept of the $\frac{dV}{d(\ln I)}$ vs. I plot gives R_s and η respectively. On the other hand, Φ_{B0} can be determined by plotting the $H(I)$ vs. I such that

$$H(I) = R_s I + \eta \Phi_{B0} \quad (13)$$

where

$$H(I) = V - \frac{\eta kT}{q} \ln\left(\frac{I}{AA^{**}T^2}\right) \quad (14)$$

As the effect of R_s is significant in the downward curvature region of the $I - V$ characteristics (Fig. 3), it is therefore customary to select the downward $I - V$ curvature region in the evaluation of Φ_{B0} , η and R_s from the Eqs. (12) and (13). Also, η value obtained from Eq. (12) plots must be taken under consideration in the evaluation of $H(I)$ and Φ_{B0} [13, 22, 24]. The selected downward curvature voltage regions for the unirradiated, 2, 4, 6, 8 and 10 kGy gamma irradiated samples lie in the range of 0.14 – 0.25, 0.12 – 0.25, 0.32 – 0.39, 0.15 – 0.20, 0.20 – 0.35 and 0.10 – 0.25 V respectively. The respective Cheung plots are shown in Figs. 5 and 6 and obtained junction parameters from these plots are reported in Table 2.

From Table 2, one can notice discrepancies in the values of Φ_{B0} and η evaluated from the TE and Cheung model due to

Table 2 $n - \text{ZnSe}/n - \text{Si}$ IHJ parameters before and after gamma irradiation at different doses

$n\text{-ZnSe}/n\text{-Si}$	TE Model		Cheung's Model		$R_s k\Omega$
	η	Φ_{B0}	η	Φ_{B0}	
Unirradiated	2.38	0.88	2.28	0.88	175.8
2 kGy	3.32	0.75	2.29	0.75	15.3
4 kGy	3.44	0.86	2.40	0.88	76.7
6 kGy	2.68	0.79	1.90	0.79	33.2
8 kGy	3.90	0.83	3.77	0.83	32.1
10 kGy	3.07	0.76	2.85	0.76	16.1

non-consideration of R_s in TE theory Eq. (7). The Φ_{B0} of the unirradiated $n - \text{ZnSe}/n - \text{Si}$ IHJ in the present study was found to be 0.88eV with η value of 2.28. Previously, Rashmitha et al. [14], Hassun et al. [25] and Güzeldir et al. [26] have reported Φ_{B0} (η) values of 0.957 (1.756), 0.825 (2.157) and 0.779eV (1.217) respectively. It is also interesting to note that for $n - \text{ZnSe}/p - \text{Si}$ heterojunctions, the reported Φ_{B0} (η) values are 0.832 (2.910) [18] and 0.78eV (3.2) [16]. Given these values, it is evident that the overall variation of Φ_{B0} lies approximately in the range of $\pm 0.1\text{eV}$ for the present study value of 0.88eV . These observations suggest that the Φ_{B0} dependence on the type of Si substrate is rather minimal but depends on the degree of homogeneity of the junction (η) owing to differences in the processing conditions (defects) as well as lattice mismatch (Tables 1 and 2).

Similar to XRD studies, no uniform trend in the variation of junction parameters was noticed in the gamma irradiated $n - \text{ZnSe}/n - \text{Si}$ IHJs. However, as noticed from Fig. 7, the

parameters, such as RR , R_s , Φ_{B0} and displaying identical trends in their variation at different GI doses. This demonstrates the direct correlation among these parameters for GI dose. However, η (not shown) has displayed a similar trend only for the GI doses in the range of 6–10 kGy while deviated at 2 and 4 kGy GI doses. This discrepancy shows the complex nature of GI induced structural modifications in the bulk and interface properties of $n - \text{ZnSe}/n - \text{Si}$ heterojunctions. Similar irregularity in trends was reported in $\text{Al}/n - \text{Si}$ Schottky junctions due to gamma induced structural modifications by generating defects [13].

3.3 Analysis of Power Law $I - V$ Characteristics

From the above as well as reported studies, $\eta > 1$ suggests the inhomogeneous nature of the junction or simply, Schottky barrier height (SBH) inhomogeneity. The greater the value

Fig. 5 $dV/d(\ln I)$ vs. I plots of $n - \text{ZnSe}/n - \text{Si}$ IHJs before and after gamma irradiation

Fig. 6 $H(I)$ vs. I plots of n -ZnSe/ n -Si IHJs before and after gamma irradiation

of η , the greater is the SBH inhomogeneity. This inhomogeneity is mainly attributed to the role of defects, either processed or irradiation induced [13, 24, 27]. Tung [28] also pointed out that the electrical data from polycrystalline Schottky barriers have always shown clear signs of SBH inhomogeneity. This is reasonable, since TE model Eqs. (7) and (11) are based on the assumptions that SBH is homogeneous when $\eta = 1$ (free of defects) and R_s is independent of bias respectively. But the fact is, most practical junctions exhibit SBH inhomogeneity due to the role of defects or the presence of an interfacial layer. Due to this, one can always notice bias dependence i.e., $\eta > 1$ and considerable value of R_s [27–29]. Also, the I – V characteristics of the junctions should be highly asymmetric (rectifying) if dominated by SBH (or thermionic emission, TE). However, the I – V characteristics shown in Fig. 3 are not highly asymmetric (poor rectification ratio), suggesting that the charge transport is not only controlled by the TE process but also the participation of defects/interface trap states in the transport mechanism across the junction. In

other words, the departure of η from unity can be attributed to the presence of interface trap states and their participation in another transport mechanism(s) in addition to the TE process. In this view, it is necessary to account for the role of interface trap states on the I – V characteristics of n -ZnSe/ n -Si IHJs before and after GI.

Apart from the tunneling process (which usually occurs for the devices with high dopant concentration or trap states), the space charge limited current (SCLC) is a widely studied conduction mechanism in single carrier devices like Schottky or heterojunctions or organic material junctions. It is common to plot SCLC I – V profiles on a double logarithmic scale to monitor current regimes by considering the slope, m , of the I – V characteristics on a log-log scale [29], i.e.,

$$m = \frac{d \log J}{d \log V} \text{ or } J \propto V^m \quad (15)$$

Figure 8(a) shows $\log I$ – $\log V$ plots of n -ZnSe/ n -Si IHJs before and after GI. Strikingly, all the samples have

Fig. 7 Variation of Schottky barrier height (Φ_{B0}), series resistance (R_s), lattice mismatch (Δ) and rectification ratio (RR) of n - $ZnSe/n$ - Si IHJs before and after gamma irradiation

exhibited two different regions of slope m values. Usually, $m = 1$ and $m = 2$ in Regions I and II, are attributed to the ohmic and SCLC conduction mechanisms respectively [29]. As noticed, in Region I, the unirradiated sample has a m value of 1.44 which is substantially greater than unity, while that of for irradiated ones (except at 2 and 4 kGy GI dose) m values are nearly equal to unity, indicating the ohmic type of conduction mechanism. In Region II, $m = 2$ has not been observed in our

studies and therefore cannot be accounted by the ideal Mott-Gurney law of SCLC [29]. This deviation of $m = 2$ in Region II as well as neither $m = 1$ or 2 in Region I for the unirradiated samples are the clear consequences of SCLC modulated by interface defect states. For this reason, the shape of the I - V characteristics is not only controlled by the SBH (TE) but also strongly depends on the distribution of interface trap states and their participation in the SCLC mechanism.

Fig. 8 (a) log I-log V plots (b) variation of slope parameter m in the region 2 and Schottky barrier height of n - $ZnSe/n$ - Si IHJs at different gamma irradiation doses

From the above, it is clear that the SCLC mechanism modulated by defects states is dominating over TE mechanism in the $n - \text{ZnSe}/n - \text{Si}$ IHJs over the measured voltage region. It is therefore important to correlate the junction parameters of both the conduction mechanisms. In literature the plots of m (an indication of defect concentration [29]) and Φ_{B0} were plotted against radiation doses to correlate them [24]. Figure 8(b) shows the variation of slope m in Region II and Φ_{B0} before and after GI. One can notice a definite but linear trend in the correlation between m and Φ_{B0} at different GI doses. Here m represents the interface trap concentration. Thus, one can interpret these modified features as real consequences due to defects and their modification at different GI doses. It can be concluded that these defects whether intrinsic or irradiation induced are responsible for poor rectification properties of $n - \text{ZnSe}/n - \text{Si}$ IHJs. However, one must note that the above conclusions are applicable only for polycrystalline $n - \text{ZnSe}/n - \text{Si}$ and cannot be generalized for single crystalline ZnSe/Si IHJs. In fact, in the latter case one may anticipate substantial improvements in the ideality factor and better rectification properties for device applications. Also, the degree of radiation induced modifications on the junction properties may remarkably vary.

4 Conclusions

A high purity ZnSe thin film was deposited onto the $n - \text{Si}$ substrate by thermal evaporation technique. The XRD studies revealed the nanocrystalline nature of the deposited ZnSe thin films with prominent (111) orientations. The $\text{Co} - 60$ gamma irradiation (GI) at different irradiation doses have shown no crystallographic phase transformations up to the GI dose of 10 kGy . However, noticeable and inconsistent variations in the ZnSe lattice parameters such as lattice constant (a), crystallinity (D), lattice strain (ϵ), dislocation density (δ) and lattice mismatch (γ) were observed at different GI doses due to gamma induced structural modifications by generating defects. The analysis of $I - V$ characteristics of $n - \text{ZnSe}/n - \text{Si}$ isotype heterojunctions (IHJs) revealed that Schottky barrier height (Φ_{B0}) dependence on the type of Si substrate is minimum (within the value of $0.88 \pm 0.10\text{ eV}$), but rather depends on the degree of homogeneity of the junction (η) due to the differences in the processing conditions, lattice mismatch (γ) and defects. The power law characteristics at different GI doses establishes linear correlation among the junction parameters such as slope parameter m , Φ_{B0} and η . It is therefore suggested that the poor rectification property of IHJs is essentially contributed by the intrinsic and gamma-induced defects and their significant role in the SCLC mechanism.

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Declarations

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