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In this paper, the influence of gamma irradiation on the structural and electrical properties of ZnSe/n-Si heterojunction is presented. The ZnSe films were deposited on n-Si (100) substrate by using thermal evaporation technique. The nanocrystalline nature of ZnSe films is confirmed from X-ray diffraction (XRD) analysis. The ZnSe/n-Si heterojunctions were subjected to gamma radiation at different irradiation doses in the range 2-10 kGy. After gamma irradiation, variations in the lattice constant, crystal size, strain and dislocation density are noticed. As a result, significant modifications in the I-V characteristics of the ZnSe/n-Si heterojunction as well as the junction parameters such as barrier height (ΦB), ideality factor (n) and series resistance (R_s) are greatly affected. An in-depth analysis of I-V characteristics is carried out by applying the graphical Cheung model and the analytical method of least squares. From these studies, it is found that ΦB and lattice mismatch between the (111) oriented ZnSe film and the (100) oriented n-Si substrate showed similar trend before and after gamma irradiation. Thereby indicating the direct dependence of ΦB on the lattice mismatch due to gamma induced defect states.

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Highlights

- Significant modifications in the structural and junction parameters of ZnSe/n-Si heterojunction is noticed after gamma irradiation.
- A direct dependence of barrier height (Φ_B) on the lattice mismatch of ZnSe/n-Si heterojunction is noticed for different irradiation doses.

Low dose gamma induced effects on structural and electrical properties of ZnSe/n-Si heterojunction

Indudhar Panduranga Vali [a], Pramoda Kumara Shetty [a,*], M G Mahesha [a], Rashmitha Keshav [a], M Rajeshwari [a], K S Vaishnavi [a]

[a] *Department of Physics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal-576 104, India*

*Corresponding author (E-mail): pramod.shetty@manipal.edu (Pramoda Kumara Shetty).

Abstract

In this paper, the influence of gamma irradiation on the structural and electrical properties of ZnSe/n-Si heterojunction is presented. The ZnSe films were deposited on n-Si (100) substrate by using thermal evaporation technique. The nanocrystalline nature of ZnSe films is confirmed from X-ray diffraction (XRD) analysis. The ZnSe/n-Si heterojunctions were subjected to gamma radiation at different irradiation doses in the range 2-10 kGy. After gamma irradiation, variations in the lattice constant, crystal size, strain and dislocation density are noticed. As a result, significant modifications in the I-V characteristics of the ZnSe/n-Si heterojunction as well as the junction parameters such as barrier height (Φ_B), ideality factor (n) and series resistance (R_S) are greatly affected. An in-depth analysis of I-V characteristics is carried out by applying the graphical Cheung model and the analytical method of least squares. From these studies, it is found that Φ_B and lattice mismatch between the (111) oriented ZnSe film and the (100) oriented n-Si substrate showed similar trend before and after gamma irradiation. Thereby indicating the direct dependence of Φ_B on the lattice mismatch due to gamma induced defect states.

Keywords: ZnSe; Gamma irradiation; Barrier height; Lattice mismatch; I-V characteristics

1. Introduction

Zinc selenide (ZnSe) is an important material of the zinc chalcogenides family. Due to its wide band gap (2.7 eV) and intrinsic n-type conductivity, it has number of applications in the field of optoelectronics including blue LEDs and lasers [1], thin-film solar cells [2], second harmonic generation [3] and nonlinear switching [4]. Despite considerable interest in the photo luminescent and electroluminescent properties of ZnSe, relatively few reports are available on electrical transport and heterojunction properties [5-11].

Fundamentally and technologically, the growth of ZnSe thin films on Si is attractive by considering the possibility of monolithic integration of ZnSe optical devices with Si electrical devices. However, the understanding ZnSe/Si heterojunction is challenging due to dissimilar thermal expansion and distinct chemical properties. Only few reports on ZnSe/n-Si and n-ZnSe/p-Si heterojunction properties are available and these studies are focused on the growth and structural characterization of the ZnSe thin films on n-Si or p-Si substrates and in few, the junction I-V characteristics is also presented [6-12].

In the recent years ZnSe nanowire/Si diode structures [13] and potential applicability of the ZnSe/Si barriers for the magnetic tunnel junctions are slowly gaining the attention [14]. However, the junction behavior of n-ZnSe/n-Si and n-ZnSe/p-Si structures are still far from being thoroughly described and/or understood. Among a variety of strategies such as thermal annealing, electron beam irradiation, inserting a layer of different semiconductor or polymer [15, 16], the gamma irradiation is quite simple technique in modifying and understanding the fundamental behavior of thin film heterojunction properties. In this view, the present article discusses on the low dose gamma induced effects on the structural and electrical properties of the n-ZnSe/n-Si heterojunction.

2. Methodology

Phosphorus doped Si <100> wafer (n-Si) having doping concentration $1.5 \times 10^{14} \mathrm{cm}^{-3}$ was procured from Sigma Aldrich, India. The ZnSe thin film were then deposited on the cleaned and diced Si wafers of dimension 0.5×0.5 cm by thermal evaporation technique. The deposition is carried out at the rate of 2 Å/s. A base pressure of 8×10^{-6} mbar was maintained during deposition. The thickness of the ZnSe thin film is kept at ~ 100 nm with the help of quartz crystal monitor. Prior to the deposition process, the n-Si wafers are cleaned according to the standard procedures [17].

The as-prepared n-ZnSe/n-Si heterojunctions are subjected to gamma irradiation using ^{60}Co source, which emits the photons of two energies (1.17 MeV and 1.33 MeV). The gamma irradiation was carried out at Centre for Applications for Radioisotope and Radiation Technology (CARRT), Mangalore University, India. The dose rate of the ^{60}Co source during irradiation was 2.6 kGy/hr. The n-ZnSe/n-Si heterojunctions are exposed to the different gamma doses of 2 kGy, 4 kGy, 6 kGy, 8 kGy and 10 kGy at room temperature. The X-ray diffraction (XRD) and junction current-voltage (I-V) characteristics studies have been carried out using Rigaku Miniflex–600 diffractometer (Cu-kα: 1.5402 Å) and Keithley source meter 2450 respectively.

3. Results and discussion

3. 1. XRD analysis

Figure 1 shows the (111) reflections of the ZnSe before and after gamma irradiation. From the various reports it is well established that thermally evaporated ZnSe films generally crystallizes in cubic zinc-blende structure having prominent (111) orientation [6-12]. After gamma irradiation, the modification in the structural parameters are clearly evidenced from the variations in the peak positions and peak widths. The parameters such as lattice constant (a), crystallite size (D) and lattice strain (ε) and dislocation densities of ZnSe thin films are evaluated by using the following relations [7]:

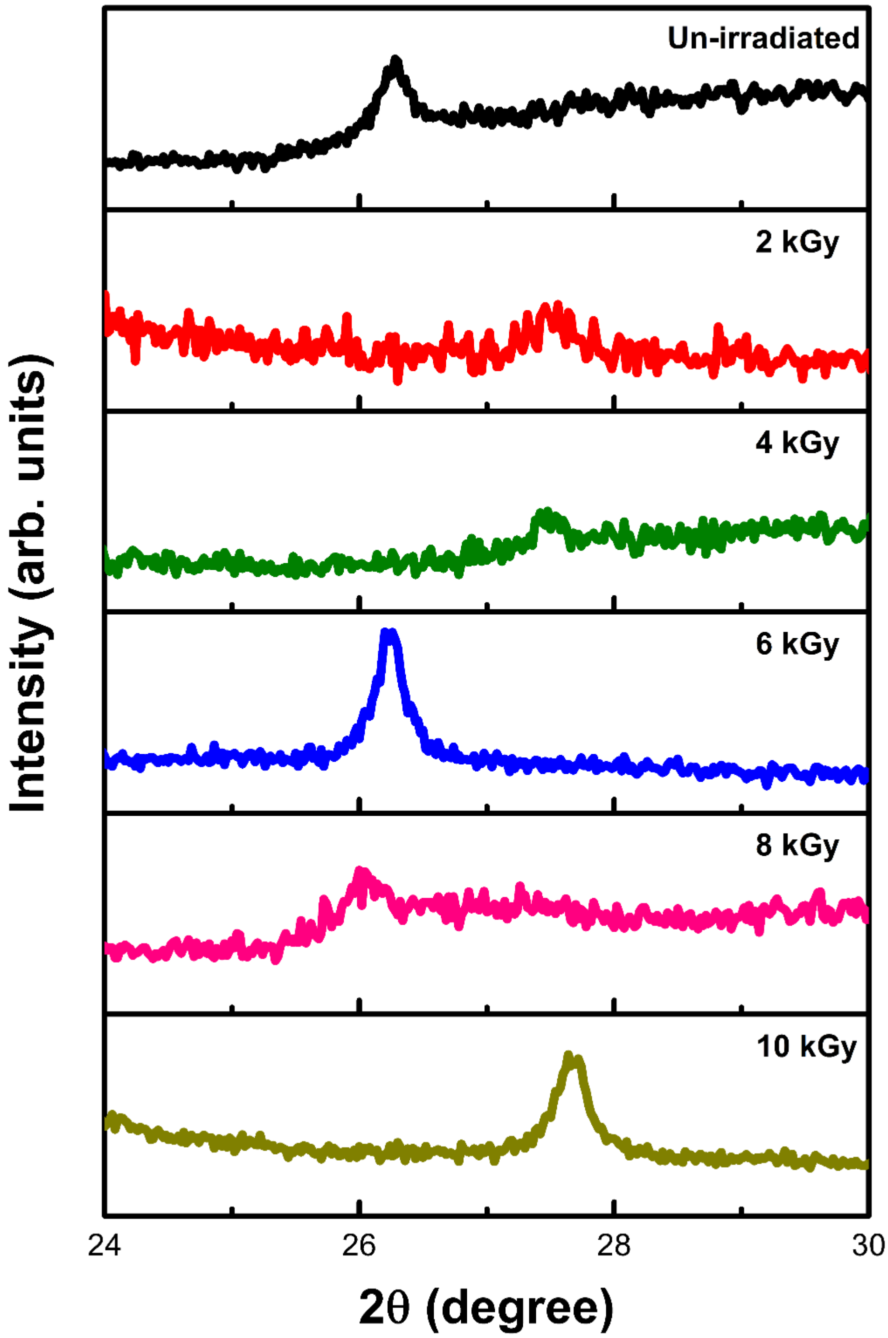

Figure 1: (111) reflection of ZnSe thin films on n-Si (100) substrate before and after gamma irradiation.

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \tag{1}$$

$$D = \frac{0.94\lambda}{\beta \cos\theta} \tag{2}$$

$$\varepsilon = \left[\frac{\lambda}{D\cos\theta} - \beta\right] \times \frac{1}{\tan\theta} \quad (3)$$

$$\delta = \frac{15\varepsilon}{aD} \quad (4)$$

where ?? = 1.5406 Å (wavelength of Cu-kα), θ is the Bragg angle and β is the full width at half maximum in radians. The variation in these parameters at different gamma irradiation is shown in Figure 2. The anamaouls variation in these parameters are attributed to gamma induced defect states and strain via ionization and displacement damage mechanisms [16, 17].

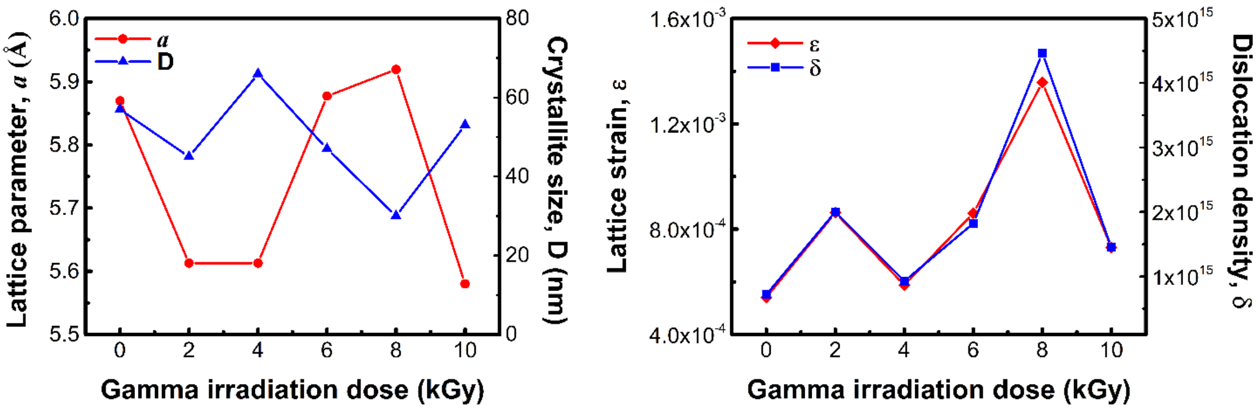

Figure 2: Variation of structural parameters of n-ZnSe thin fims on n-Si (100) substrate before and after gamma irradiation.

3. 2. Analysis of I-V characteristics

Figure 3 shows the I-V characteristics of n-ZnSe/n-Si heterojunction before and after gamma irradiation. As noticed the junction is exhibiting rectifying characteristics with small rectification ratio. As observed, the I-V characteristics are sensitive to the gamma irradiation dose. To understand the junction properties at different irradiation doses, the contact parameters must be determined. The barrier height (Φ_B) of the junction is usually determined by applying classical thermionic emission (TE) model. However, Φ_B determined from the TE model does not takes into the account of the barrier inhomogeneity (which is modelled as n, known as ideality factor) and the voltage drop across the thin insulating medium (which is modelled as R_S, known as series resistance). There exist different approaches to evaluate Φ_B in consideration of n and R_S from the I-V characteristics. In the present paper we applied different approaches to evaluate these parameters and the results are compared. First, we applied graphical functions proposed by Cheung and Cheung, also known as Cheung model [18] and second we applied the method of least squares proposed by Bennett [19]. The outline of these two methods is given below.

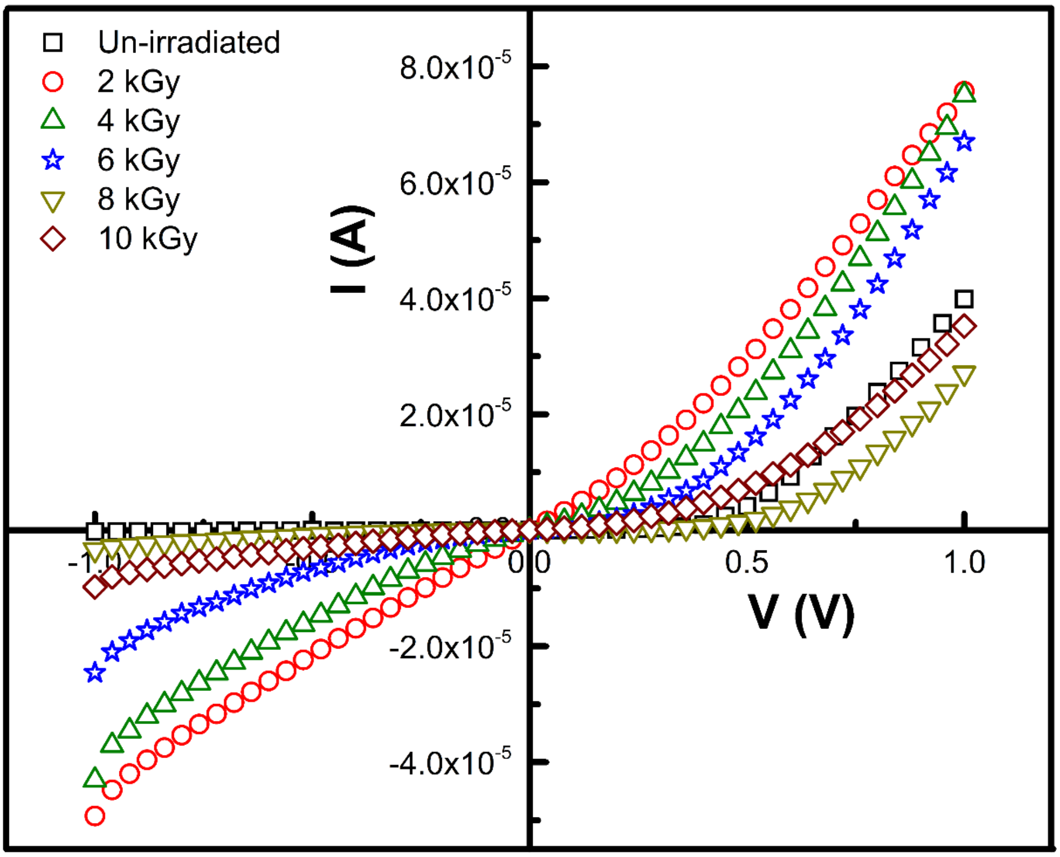

Figure 3: I - V characteristics of un-irradiated and irradiated ZnSe/n-Si hetero-structures

3. 2. 1 Cheung model

For the applied voltage $V > 3kT/q$, the TE model equation in consideration of n and R_S takes the form,

$$I = I_S \exp\left[\frac{q(V - IR_S)}{nkT}\right] \tag{5}$$

$$\text{where } I_S = AA^{**}T^2 \exp\left(-\frac{q\Phi_B}{kT}\right) \tag{6}$$

k is Boltzmann constant, T is absolute temperature, A is device area, A^{**} is Richardson constant (for n-Si, $A^{**} = 112\ A \cdot cm^{-2}K^{-2}$ [20])

The differentiation of Eq. (5) with respect to I gives the relation,

$$\frac{dV}{d(\ln I)} = R_s I + \frac{nkT}{q} \qquad (7)$$

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

$$H(I) = R_s I + n\Phi_B \qquad (8)$$

$$\text{where } H(I) = V - \frac{nkT}{q}\ln\left(\frac{I}{AA^{**}T^2}\right) \qquad (9)$$

In plotting the Cheung functions (7) and (8), the downward curvature of the I-V characteristics must be selected. The Cheung plots of n-ZnSe/n-Si heterojunction before and after gamma irradiation is shown in Figure 4 and the obtained parameters are reported in Table 1.

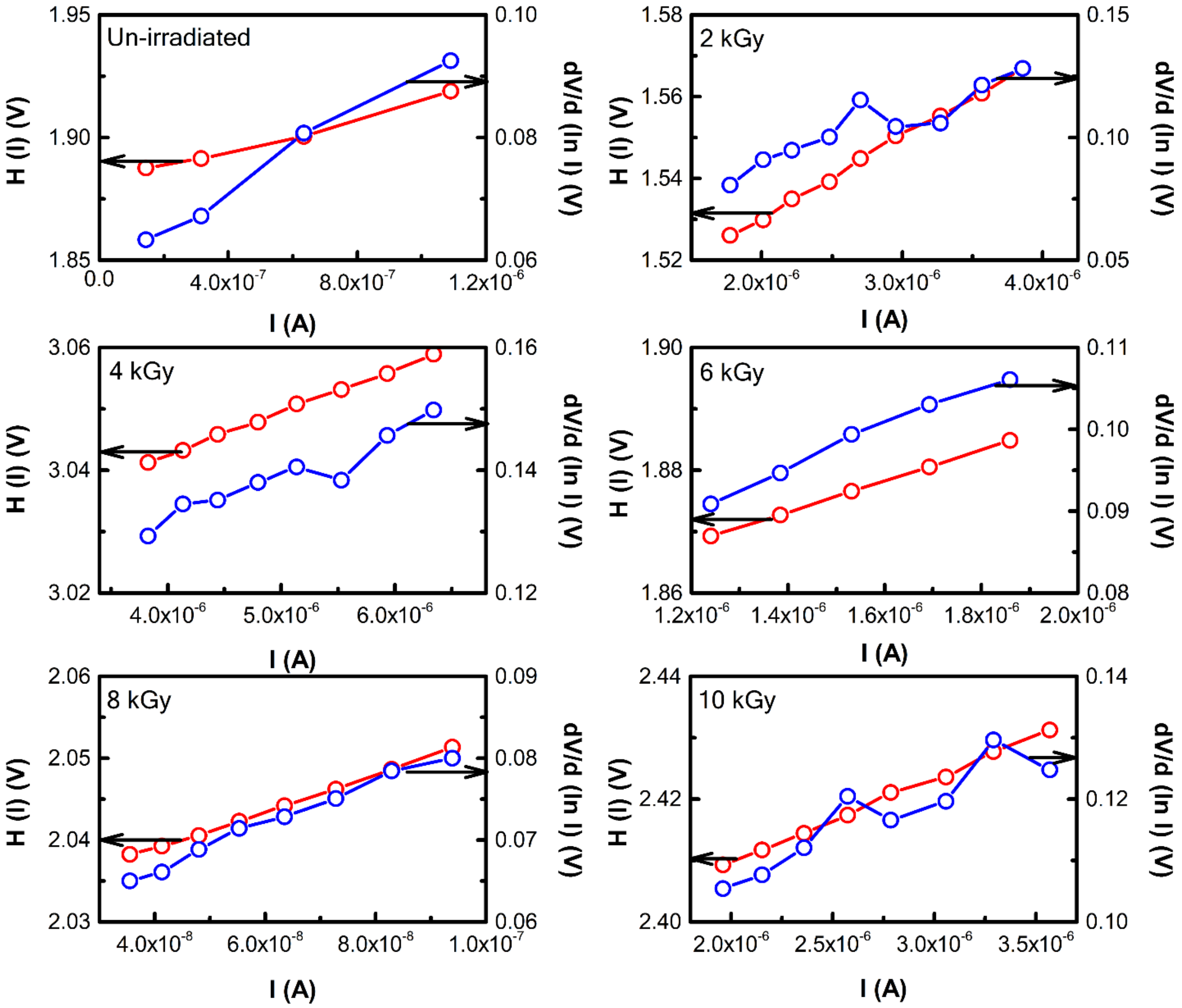

Figure 4: Cheung plots of n-ZnSe/n-Si heterojunction before and after gamma irradiation.

Table 1. n-ZnSe/n-Si heterojunction parameters before and after gamma irradiation at different doses.

n-ZnSe/n-Si	Cheung Model			Method of least squares		
	Φ_B (eV)	n	R_s (kΩ)	Φ_B(eV)	n	R_s(kΩ)
Un-irradiated	0.83	2.26	32.59	0.86	2.85	8.95
2 kGy	0.76	1.96	19.64	0.71	3.32	9.15
4 kGy	0.75	4.01	7.01	0.73	4.19	7.22
6 kGy	0.79	2.33	25.15	0.76	3.99	6.81
8 kGy	0.89	2.26	26.44	0.87	3.18	10.79
10 kGy	0.77	3.09	13.69	0.77	4.65	12.01

3. 2. 2 Method of least squares

Eq. (5) can be re-written as

$$V = IR_s + \frac{nkT}{q}\ln\left(\frac{I}{I_s}\right) \tag{10}$$

substituting $\frac{nkT}{q} = a$ and $-\frac{nkT}{q}\ln I_S = b$ (11)

we obtain the simplified expression as

$$V = IR_s + a\ln I + b \tag{12}$$

Eq. (12) define the actual current I when the voltage V is applied across the junction.

The unknown parameters a, b and R_s can be optimized by the method least squares by defining

$$S = \sum_{i=1}^{m}\{I_i R_s + a\ln I_i + b - V_i\}^2 \tag{13}$$

Here the summation is over m experimentally observed data pairs of V and I. The ideal combination of the parameters a, b and R_s would result in minimum S when

$$\frac{\partial S}{\partial R_s} = \frac{\partial S}{\partial a} = \frac{\partial S}{\partial b} = 0 \tag{14}$$

Then the obtained set of equations in the matrix form $AX = B$ is written as

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix}\begin{bmatrix} R_s \\ a \\ b \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} \tag{15}$$

where $c_{11} = \sum_{i=1}^{m} I_i^2$; $c_{12} = c_{21} = \sum_{i=1}^{m} I_i \ln I_i$; $c_{13} = c_{13} = \sum_{i=1}^{m} I_i$; $c_{22} = \sum_{i=1}^{m} (\ln I_i)^2$;

$c_{23} = c_{32} = \sum_{i=1}^{m} \ln I_i$; $c_{33} = m$; $f_1 = \sum_{i=1}^{m} I_i V_i$; $f_2 = \sum_{i=1}^{m} V_i \ln I_i$; $f_3 = \sum_{i=1}^{m} V_i$ (16)

Therefore, the parameters Φ_B, n, and R_s can be determined by solving Eq. (15). The evaluated values of the parameters are reported in Table 1.

As noticed, the contact parameters obtained from the Cheung model and the method of least squares are different. This is due to the region in which the parameters are extracted. In the case of Cheung model, the parameters are extracted by selecting the voltage region in the downward curvature region of the forward I-V characteristics (Figure 1). But in the case of method of least squares the entire forward voltage is considered in extracting the parameters. Thus the parameters derived from the method least squares gives the average value over the entire I-V characteristics. The greater than unity ideality factors before and after gamma irradiation is an indicative of the barrier inhomogeneity [15-17]. In addition, the power law characteristics (not given) also showed that the slope parameter $m > 2$, which is an indicative of exponential distribution of trap states over the entire region. Therefore, the thermionic emission of electrons over the barrier and the space charge limited emission mechanisms are the competing transport mechanisms over the entire voltage region. In addition to these, the tunneling and tunneling through the trap states could be also expected to take place at lower forward voltages [16, 17].

The contact parameters can be easily correlated with the lattice mismatch of the ZnSe/n-Si junction. The percentage of lattice mismatch (Δ) between the (111) oriented ZnSe film and (100) oriented Si substrate is evaluted by using the relation

$$\Delta = \frac{a_{ZnSe} - a_{Si}}{a_{Si}} \times 100\ \% \qquad (17)$$

where a_{ZnSe} and a_{Si} are the lattice parameters of ZnSe and Si respectively.

Figure 5 the shows the variation of Δ and Φ_B as a function of gamma irradiation dose. As noticed both Δ and Φ_B are exhibiting similar trend with gamma irradiation dose. This is mainly attributed to the gamma induced defect states at the junction. Similar trend is also noticed for the variation of Δ and R_s evaluated from the Cheung model (not shown). However, the R_s evaluated from the method of least squares is slightly deviated from its correlation with lattice mismatch. This discrepancy is ascribed to the selection of voltage region between the two models.

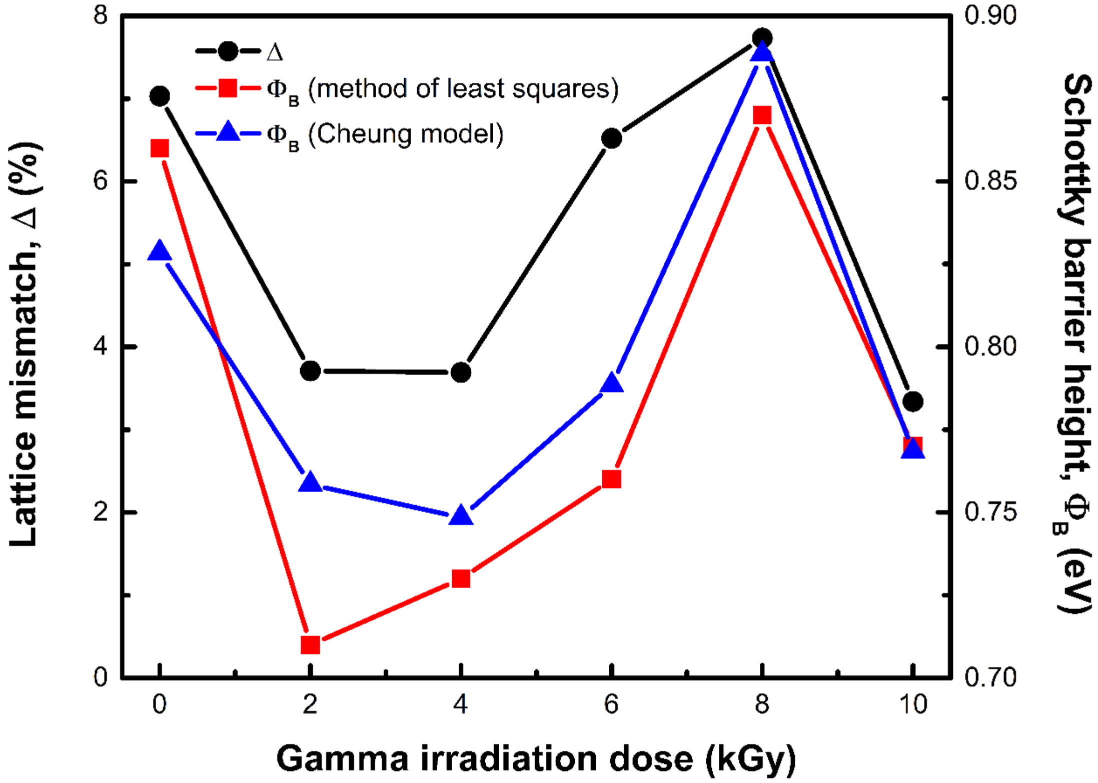

Figure 5: Correlation between lattice mismatch (Δ) and barrier height (Φ_B) of the n-ZnSe/n-Si heterojunction as a function of gamma irradiation dose.

4. Conclusion

The ZnSe thin films were deposited on the n-Si (100) substrate using thermal evaporation technique. The XRD studies showed nanocrystalline form of the deposited ZnSe thin films on n-Si substrate. The gamma irradiation on the ZnSe/n-Si heterojunction showed remarkable variations in the parameters such as lattice constant (a), crystallinity (D), lattice strain (ε), dislocation density (δ) and lattice mismatch (Δ) at different irradiation doses. The analysis of I-V characteristics by applying Cheung model and method of least squares showed that the barrier height (Φ_B) of the ZnSe/n-Si heterojunction is strongly dependent on the lattice mismatch between the (111) oriented ZnSe and (100) oriented n-Si at different gamma irradiation doses.

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