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Simulation and performance analysis of n-ZnO/p -GaSb heterojunction device

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ABSTRACT

In the present paper, attempt has been taken to study the electrical performance analysis of n-ZnO/p-GaSb heterojunction device. Prior to fabrication of this device, simulation and analysis have been carried out to avoid extensive use of time. For this purpose, ATLAS simulator tool of SILVACO International was used. The energy band diagram for this heterojunction have been drawn based on Anderson's model and found to be Type-II in nature. Current-Voltage (I-V) characteristic of the heterojunction device shows rectifying nature when analyzed for different temperature ranging from 300K to 400K. The effect of variation in temperature on the device parameters like ideality factor, barrier height and threshold voltage have also been analyzed. The ideality factor is found to be greater than one which predicts that the current transport mechanism for the present structure not only depends on thermionic emission but also on the tunnelling mechanism

Keywords:*n-ZnO/p-GaSb; Heterojunction, electrical performance; diode, SILVACO.*

1. INTRODUCTION

In the area of microelectronic integrated circuits, the device applications were based on metal-semiconductor interface [1]. For the high speed and high frequency responses Schottky contacts play a major role. The current transport across such interface is usually predominated by the thermionic emission mechanism. The performance and reliability of the Schottky barrier diode is dependent on the quality of interface between the metal and semiconductor. The applications based on Schottky contacts consisted of heterojunction bipolar transistor, heterojunction diode, photodiode, phototransistors, radio-frequency detectors etc., for such applications recently many compound semiconductors were chosen; gallium antimony (GaSb) and zinc oxide (ZnO) are two such attracting photonic materials from two different groups of compound semiconductors. Recently, GaSb is one of the III-V compound semiconductor attracted much consideration as a significant material for fabrication of optoelectronic devices operating at a wavelength range of 1~5μm. GaSb has an energy band gap of 0.70eV (1.77 μm) at room temperature (RT) and 0.81eV (1.53μm) at 4K. Its lattice constant of 6.0959 Å at room temperature (RT) matches that of various ternary and quaternary compounds with band gaps covering a wide spectral range of 0.3–1.58eV (0.8–4.3μm) [2]. Besides GaSb, Zinc Oxide (ZnO) has also attracted intense attention in research field due to its wide and direct band gap of 3.37eV with hexagonal wurtzite structure. ZnO is also a attractive semiconductor material for various electronics, optoelectronic and sensor applications. Another advantageous feature of ZnO is that it can be easily synthesized or grown on any substrate [3-5]. Furthermore, it is found that ZnO is n-type irrespective of growth condition. However, it is not easy to synthesize p-ZnO at room temperature due to the low oxygen (O) concentration in comparison to Zn. According to our knowledge, no reports available on stable and reproducible p-type ZnO sample [6]. Recently researchers have worked on electrical, structural, and optical characterizations of different heterostructures. Suleyman Tekmen et al [7] reported on the electrical, structural and optical characterizations of ZnO/GaAs heterojunction diode and N. N. Halder [8] reported on photoluminescence studies of n-ZnO/p-GaAs structure whereas M. Soylua [9] reported on the electrical characteristics of sol-gel synthesized n-ZnO/p-GaAs heterojunction. P. Koc et al, S. E. Nikitin et al and Yu. A et al reported on electroluminescence emission studies were carried out on n-ZnO/P-GaAs:Zn heterojunction fabricated by electro-deposition method using simulation method [10-12]. P. F. Zhang et al [13] reported on valance band offset of ZnO/GaAsZnO/GaAs heterojunction measured by X-ray photoelectron spectroscopy. H. Zhang reported on fabrication and characterization of high-quality n-ZnO/p-GaN heterojunction light emission diodes [14]. J Y Lee et al [15] reported on oxide defects of laser-spike-annealed ultrathin hafnium-oxide high-k dielectric stacks. S Chirakkara et al [16] reported on study of n-ZnO/p-Si (100) thin film heterojunctions by pulsed laser deposition without buffer layer. The observations from the above literature survey directed us towards the simulation and performance analysis of n-ZnO/p-GaSb heterojunction device. For the present paper, ATLAS simulator from SILVACO International has been used to save time and money. The study also reports on the effect of change in temperature on the performance of n-ZnO/p-GaSb heterojunction. Additionally, when we move from simulation study to actual fabrication; the set of device parameters with which the efficient performance of n-ZnO/p-GaSb heterojunction can be obtained.

2. DEVICE SIMULATION SETUP

A simulation program for proposed n-ZnO/p-GaSb heterojunction diode structure has been developed using ATLAS simulator from SILVACO International to obtain various electrical characteristics. The structure of the n-ZnO/p-GaSb heterojunction devices has been formulated as per the Anderson model [17]. The schematic symbol of n-ZnO/p-GaSb heterojunction is shown in Figure 1 with top and bottom contact of Aluminium (Al). A voltage from -1V to +1V is applied in an appropriate polarity as shown in Figure 1.

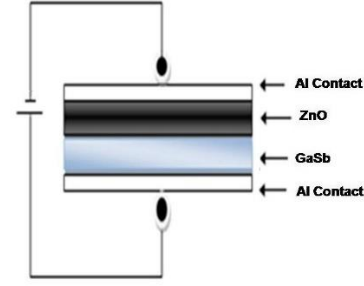

Figure 1. Schematic diagram of *n*-ZnO/*p*-GaSb heterojunction.

3. RESULTS AND DISCUSSIONS

Figure 2 shows the proposed energy band diagram for n-ZnO/p-GaSb heterojunction as per the Anderson's model and it is found to be of Type II. Initially, we defined the physical structure of the device. Afterwards the material properties of ZnO and GaSb have been defined. Some parameters used for simulation such as conduction band discontinuity (ΔE_c), Valence band discontinuity (ΔE_v), Fermi level in n-type (Φ_{fn}) and Fermi level in p-type (Φ_{fp}) semiconductor, built-in potential barrier (Φ_{bi}), Depletion width in n-region (x_n), Depletion width in p-region (x_p) , effective density of state for electron (N_c) and effective density of state for holes (N_v). The above parameters have been calculated using the following formulas:

$$\Delta E_c = q(\chi_{ZnO} - \chi_{GaSb}) \quad (1)$$

$$\Delta E_V = (E_{gZnO} - E_{gGaSb}) - \Delta E_C \quad (2)$$

$$\phi_{fn} = KTln\left(\frac{N_d}{N_c}\right) \quad (3)$$

$$\phi_{fp} = KTln\left(\frac{N_a}{N_v}\right) \quad (4)$$

$$\phi_{bi} = \frac{E_{gp}+\Delta E_C-\phi_{fp}-\phi_{fn}}{q} \quad (5)$$

$$N_c = 2\left(\frac{2\pi m_e KT}{h^2}\right)^{\frac{3}{2}} \quad (6)$$

$$N_v = 2\left(\frac{2\pi m_h KT}{h^2}\right)^{\frac{3}{2}} \quad (7)$$

Where, χ_{GaSb} and χ_{ZnO} are the electron affinities of GaSb and ZnO, E_{gGaSb} and E_{gZnO} are the band gaps of GaSb and ZnO, h is Plank's constant, K is Boltzmann constant, q is the charge of electron and T is the lattice temperature in Kelvin. Using the above formulae, all necessary parameters are calculated for the energy band diagram to be drawn.

Table 1 shows the set of material parameters (like band gap, electron affinity, dielectric constant, electron/hole mobilities, conduction band densities, valence band densities etc) for simulation and performance analysis of *n*-ZnO/*p*-GaSb heterojunction diode. All these parameters have been obtained from various literatures [3, 4, 18]. In the present study, we considered uniform doping density for both the *p* and *n* regions. To get better efficiency, we used the Newton-Gummel iteration method. For the present study, we considered AUGER, Band-to-Band tunneling and SRH model of recombination mechanism [19]. For contacts, mobility calculation and surface recombination, concentration dependent model has been considered. Finally, the current-voltage (I-V) characteristics were carried out for a voltage range from -1V to +1V at a step of 0.1V for 300 K to 400 K temperature range. The current value increases with increase in temperature.

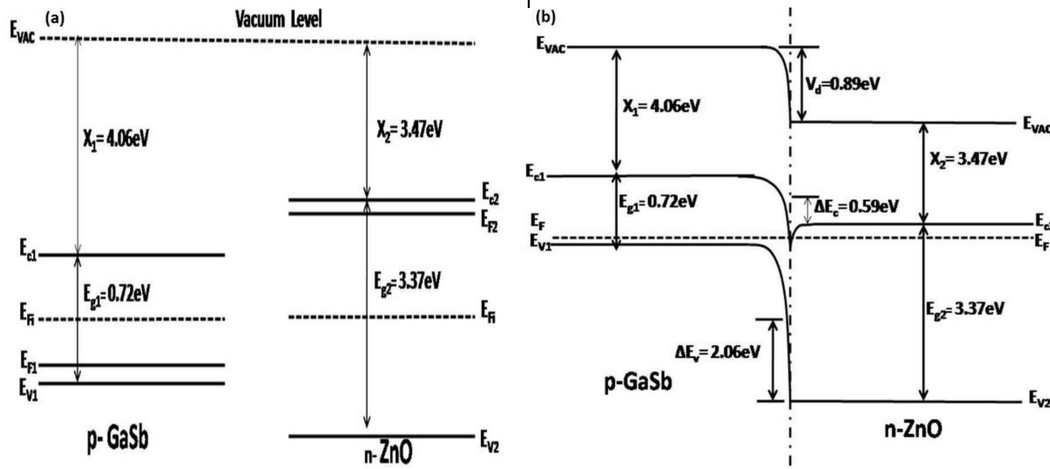

Figure 2. Schematic diagram of the Energy band diagram of *n*-ZnO/*p*-GaSb heterojunction (a) before joining (b) after joining.

Table 1. Values of material parameters used for simulation of n-ZnO/p-GaSb heterojunction.[3,4,18]

Parameter	Value
Electron Affinity, χ (eV)	4.06 (χ_{GaSb}) 3.47 (χ_{ZnO})
Bandgap, E_g (eV)	0.72 (E_{gGaSb}) 3.3(E_{gZnO})
Dielectric constant, Є	15.2 ($Є_{GaSb}$) 8.5 ($Є_{ZnO}$)
Donor Concentration, N_D (cm^{-3})	2.18×10^{18}
Acceptor Concentration, N_A (cm^{-3})	3.17×10^{17}
Electron mobility, μ_e (cm^2/V.sec)	4000 (GaSb)
Hole mobility, μ_h (cm^2/V.sec)	1400 (GaSb)
Effective density of states in the conduction band, N_c(cm^{-3})	1.76×10^{18} (GaSb) 2.2×10^{18} (ZnO)
Effective density of states in the valence band, N_v(cm^{-3})	8.87×10^{18} (GaSb) & 1.8×10^{19} (ZnO)

The current-voltage characteristics were measured to obtain the effective values of the diode parameter. Figure 3 show the current-voltage characteristic of n-ZnO/p-GaSb heterojunction, which shows rectifying diode characteristic and the current increases exponentially with a very low value of applied voltage. At a reverse bias of -1V relatively low reverse current of 0.089×10^{-9} A has been obtained.

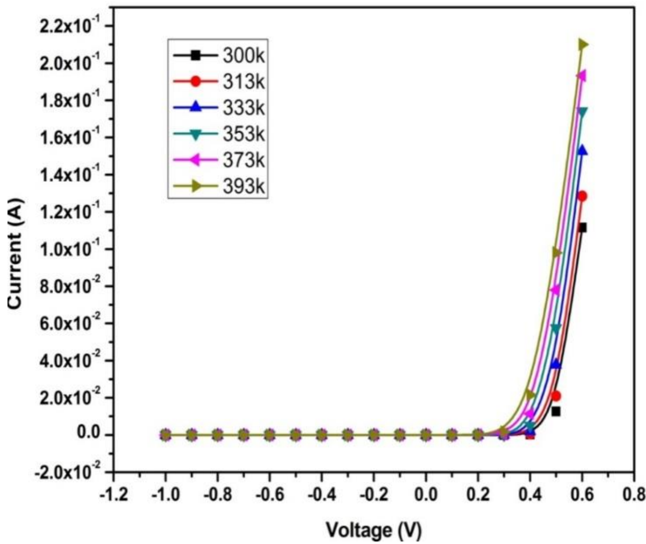

Figure 3. I-V characteristic of n-ZnO/p-GaSb heterojunction.

The current flow for the proposed structure can be analyzed by considering the thermionic emission theory as given by [17, 19-21].

$$I = I_s exp\left(\frac{qV}{\eta KT} - 1\right) \quad (8)$$

Where, V is the applied voltage and I_s is the reverse saturation leakage current which is found to be

$$I_s = AA^*T^2 exp\left(\frac{q\phi_b}{KT}\right) \quad (9)$$

Where, q is the electronic charge, A is contact area, A* is the effective Richardson constant, K is the Boltzmann's constant, T is the absolute temperature, Φ_b is the barrier height and η is the ideality factor. The value of Φ_b and η were calculated (according to the thermionic emission theory as function of time) from the intercept and slope of the forward bias ln(I) versus voltage (V) plot is as shown in Figure 4. Therefore, the slope (m) of the forward bias lnI vs Voltage characteristic is given by,

$$m = \frac{lnI_2 - lnI_1}{V_2 - V_1} \quad (10)$$

The slope obtained will give the ideality factor as

$$m = \frac{q}{\eta KT} \quad (11)$$

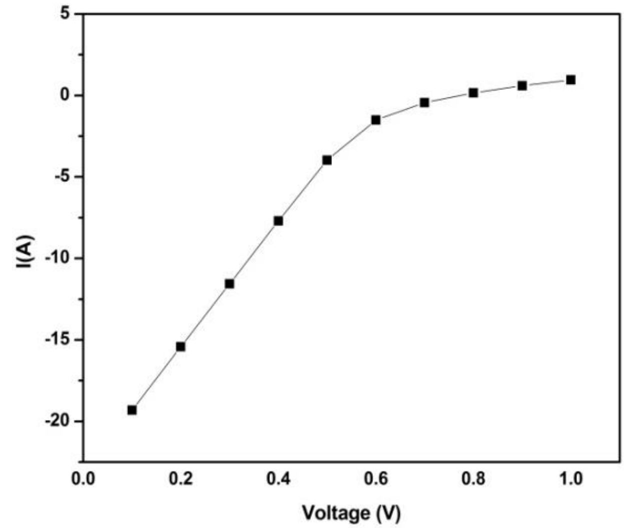

Figure 4. ln I vs Voltage of n-ZnO/p-GaSb heterojunction diode at 300K.

The Figure 5 shows the effect of ideality factor obtained by varying the temperature. It is observed that ideality factor decreases with increase in temperature. The ideality factor found greater than unity at 300K implies that recombination current may be present in the proposed device. For the present case, the current transport mechanism cannot be explained by thermionic emission only; there may be presence of secondary transport mode existing like tunneling mechanism [19-22].

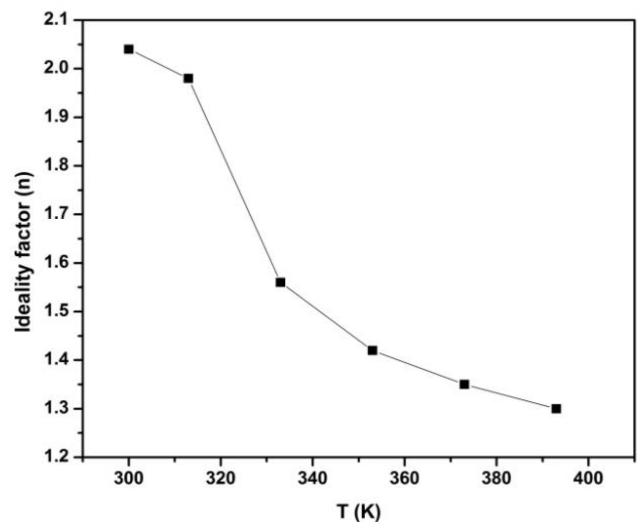

Figure 5. Temperature dependence of ideality factor of n-ZnO/p-GaSb heterojunction.

From ln (I) vs Voltage plot, by extrapolating the linear line upto the Y-axis, the intercept obtained at Y-axis gave the barrier height. The Figure 6 shows the effect of barrier height calculated

for different temperature which increases with increase in temperature.

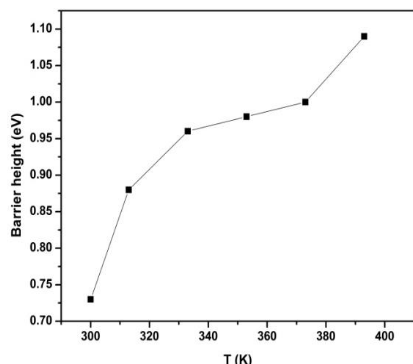

Figure 6. Temperature dependence of barrier height of n-ZnO/p-GaSb heterojunction.

In case of a metal-semiconductor junction, the transport mechanism explains that even at low temperature for a higher ideality factor electrons can overcome the barriers to contribute in the conduction mechanism. With the increase of temperature, more and more electrons acquire energy to overcome the barriers. Thus, with rise in temperature the threshold voltage is expected to decrease [20-24]. The similar conditions are happening in case of our proposed n-ZnO/p-GaSb heterojunction device. Threshold voltage is the point where the current starts to increase in the forward bias direction. From the I-V characteristic for different temperatures it is found that the threshold voltage decreases with the increase in temperature as shown in Figure 7. This may be affected the depletion width at the interface supporting the secondary transport mechanism to exist at higher temperature [7].

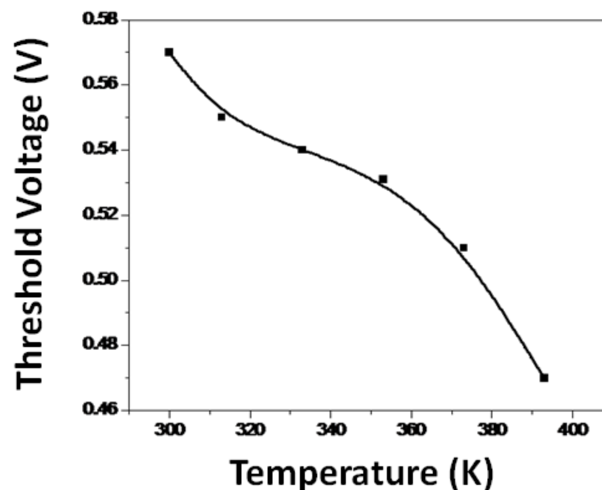

Figure 7. Temperature dependence of threshold voltage of n-ZnO/p-GaSb heterojunction.

4. CONCLUSIONS

The simulation and performance analysis of n-ZnO/p-GaSb heterojunction diode is studied using ATLAS simulator from SILVACO International. The energy band diagram of the proposed heterojunction has been drawn basing on Anderson's model and found to be Type II in nature. Important parameters like ideality factor, barrier height, and threshold voltage have been obtained from the current-voltage characteristic curve measured at room temperature and also the effects of change in temperature on these parameters have been studied.The greater than one value of ideality factor, variation of threshold voltage and barrier height assumes the current transport mechanism at the n-ZnO/p-GaSb heterojunction device interface is not only due to the thermionic emission but also may be due to the tunneling mechanism. The present study and analysis paper suggests the set of device parameters with which the efficient performance of n-ZnO/p-GaSb heterojunction can be obtained before moving for actual fabrication.

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