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NUMERICAL INVESTIGATION OF CURRENT TRANSPORT PROPERTIES OF FUTURE GENERATION DEVICE UNDER HIGHLY SENSITIVE TEMPERATURE

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In present research, current-transport mechanism in future generation devices like Schottky diodes under highly sensitive temperature was investigate through the mathematical approach. Typical thermionic emission model and Cheung function were taking into account for analysis of transportation mechanism in a Schottky diode in forward bias. Different electrical parameters were calculated for analysis of temperature variation effect. Simulation of electrical parameters was performed via MATLAB under the sensitive temperature range from 300K-1000K. Obtained results showed that barrier height and ideality factor are strongly temperature dependent. The barrier height was inversly proportional while the ideality factor was directly proportional to the temperature.

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Keywords: Temperature effect, Electrical properties, Future generation devices, Thermionic emission model, Cheung function

1. Introduction

The field of Nano science and Nano technology has been seeking to develop new and improved devices that have the capability to improve the life quality of human beings. Researchers have intensively devoted themselves to work in this area of research and are continuously trying to fabricate Nano scale devices with improved performance to make human life easier [1]. Nanotechnology is one of the leading fields that are creating new opportunities to make human life safer and secure by fabricating nanoscale devices [2-3]. But the more use of electronic devices will create more demand of energy. Therefore it is very important that these nanoscale devices are not only smaller in size, more functional and easy to manufacture but must be less toxic, biosafe, biodegradable, biocompatible and low consumption energy devices [4-5]. Beside this the improvement in the performance of these electronics devices is also vital and the scientists/researchers tried hard in this aspect as well. The improved performance of the electronics devices can be achieved in many ways, but the most important is by utilizing the electrical and mechanical properties. Many self powered and low powered devices have been fabricated in last two decdes by manipulating electrical properties of different materials. Park et al described the current transport mechanism in Light-emitting diodes [6],Huang et al. introduced UV nanolasers[7], Soci et al. invented UV photo detectors [8], Arnold et al. fabricated field-effect transistors[9] and Buchine et al. discovered piezoelectric transducer/actuator[10] . The mechanical properties of different materials are also very critical as far as improved performance of nanoscale devices is concerned and this can be achieved by manipulating different parameters such as barrier height, ideality factor, series resistance etc [11-13]. Among many electronic applications Schottky diodes are one of the most simplest and extensively used electronic device. To obtain high performance of Schottky devices the selection of material is very crucial. Because of wide band gap different semiconductors have been studied in this reagrd but Zinc Oxide (ZnO) became the most extensively studied semiconducting material for the fabrication of electronic devices due to its excellent electrical, mechanical and piezoelectric properties [14]. Beside this ZnO has diversity of nanostructures, such as nanorods, nanoflowers, nanowires, nanobelts, nanoneedles, nanoflakses etc [15]. By using specific growth conditions it is possible to synthesize one-dimensional ZnO nanostructures which can produce high potential, which is useful in fabrication of superior

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nanoscale devices. ZnO is also a good candidate for power semiconductor devices because it has excellent electrical properties and thermal stability which are very important for high voltage, high power, high temperature devices. The direct wide bandgap (3.37eV), high thermal conductivity and large exciton binding energy of 60meV are also very promising features of ZnO [16]. Beside these high electron saturation velocity and high resistance radiation are some other appealing properties of ZnO to work on [17].

Now in order to prepare high performance of Schottky devices, it is also important to form high quality Schottky contacts on ZnO [18]. The Schottky diode, also known as Schottky barrier diode or hot-carrier diode is a semiconductor diode formed by the junction of a semiconductor with a metal. It is established that high work function noble metals like Platinum (Pt), Gold (Au) and Palladium (Pd) can form excellent Schottky contact with ZnO nanostructures [19]. The ZnO Schottky contact was first published by Mead et al. [20], Yadav et al.reported the Pd Schottky contact on ZnO using sol-gel technique [21], Aydo˘gan et al. used electro-deposition technique to fabricate Au/n-ZnO Schottky diodes on n-type silicon substrate and investigated its electrical characteristics [22], Periasamyet al. has studied Pt contact on ZnO thin film using vacuum evaporation and thermal evaporation technique [23].Since the quality of Schottky devices depend on the inhomogeneities, series resistance and insulating layer between metal and semiconductor interface [24], therefore the barrier height, ideality factor and series resistance are important parameters in this regard. It is well established that Schottky contacts showed strong dependence of temperature with these factors [12-13].

The most influenced factors in a Schottky diode are barrier height and ideality factor. Most of the researchers investigated electrical properties of Schottky diode based on post annealing but few reported below the room temperature [25]. Allenet et al. determined the Schottky barrier height (0.77 eV) and the ideality factor (1.1) for Ag–ZnO-based diode [26]. Osval et al. studied the GaN Schottky diodes with two crystal polarities (Ga- and N-face) and reported that barrier height is decreasing with decrease in temperature and ideality factor is increasing. Akkal et al. studied the current-voltage characteristics of Au/n-GaN Schottky diodes in the temperature range 80K-300K and reported ideality factor (1.18) at room temperature [27-28]. M Asghar et al. Calculated barrier height (0.68 eV) and ideality factor (2.68) for Au/ZnO/Si diode at temperature range of 150K-400K [29].Gullu et al. obtained ideality factor and barrier height for Al/DNA/Si diode in the temperature range of 200K-300K as 1.34 ± 0.02 and (0.75 ± 0.01) eV at 300K and 1.70 ± 0.02 and (0.61 ± 0.01) eV at 200K respectively. It was observed that the Schottky barrier height increases with temperature and at high temperature the diode showed the non ideality [30]. Somnath Mahato et al. has investigated electrical parameters of Au/V_2O_5/n-Si Schottky diode by Current-Voltage (I-V) and Capacitance-Voltage (C-V) characterstics in the temperature range of 150K to 300K and found the values of ideality factor and barrier height as 2.04 and 0.83 eV at 300 K and 6.95 and 0.39 eV at 150 K respectively[31]. Beside this I-V and C-V characterstics are widely used to study the influence of temperature on barrier height and ideality factor of Schottky diodes with different ranges of temperature[29].

It is an established fact that experimental study is always costly and time consuming. Therefore numerical investigations can play an important role in this regard. In literature, several numerical methods have also been discussed for extraction of Schottky diode parameters and these results have showed enough accuracy and high degree of certainty/assurance [32]. Durmuş Ali Aldemir et al. measured barrier height and ideality factor of Ni/n-GaAs Schottky diode by using conventional I-V method, Norde method, generalized Norde method and Cheung function in the temperature range of 60K to 320K [33]. M. Khalid et al. determined Schottky barrier diode characteristics of Pt/SiC by using Sentausurs TCAD tools [34]. But to the best of authors knowledge and belief niether experimental nor any numerical work has been conducted as yet beyond the temperature range of 673K.

This study mainly deals with numerical investigation of electrical parameters of ZnO based Schottky diode in the temperature range of 300K-1000K. This investigation has been performed by using MATLAB programing. The simulation program produced acceptable range of parameters magnitudes with additional advantage of accurately modeled physical parameters in forward bias. Numerically obtained results of ZnO based Schottky diode in the temperature range of 300K-1000K have also been compared by using thermionic emission model(T.E.M.) and Cheung function(C.F.) to find the barrier height and ideality factor.

2. Theoretical models

The I-V and C-V describes the transport properties of a Schottky diode and inverse surface layer showed strong influence on the transport properties of a Schottky diode [35]. ZnO based Schottky diode was considered to determine the transport properties numerically and two different models were used for comparison of results in the temperature range of 300K-1000K. A typical T.E.M. shown in equation (1) was used for the calculation of electrical parameters of Schottky diode.

$$I = Pe^{Q(V-n\varphi_b)} - Pe^{-Qn\varphi_b} \tag{1}$$

Where

$$P = AR^*T^2 \; and \; Q = \frac{q}{nKT}$$

2.1. Typical T.E.M.

It is well known that, the mechanism of current transport in a Schottky diode can be defined by standard T.E.M. as shown in equation (1), while saturated current I_o is expressed in equation (2).

$$I_o = AR^*T^2e^{-\frac{q\emptyset_b}{KT}} \tag{2}$$

Here K is Boltzmann constant,T is temperature in Kelvin, A is the area of Schottky contact and R is Richardson constant for ZnO (32 A/cm^2K^2), n is an ideality factor and $\emptyset_b$is the barrier height of the Schottky diode.

The I-V characterstics of ZnO based Schottky diode in the temperature range of 300K-1000K are shown in Figure 1. It can be clearly seen in Figure 1(a) that the exhibited nonlinear exponential rise and the built-in potential is in the range of 0.6-1.0. Moreover, it is clear from Figure 1(a) that, the built-in potential is decreasing with rise in temperature. This variational effect might be due to the low resistance against the rising values of the temperature, because the reverse saturation current is almost $8.36x10^{-8}$A, showing the weak resistance. The calculated values of the ideality factor, barrier height, buitl-in potential and the reverse saturation current via T.E.M. are slightly different than the values calculated throught the C.F.. But all these values have good consistancy with previously published experimental work [36]. In Figure 1(b) the intercept of linear portion of lnI-V curves used to obtain the values of saturated current. Whereas the values of barrier height of Schottky diode were calculated by using the calculated values of saturated current in equation (3).

$$\emptyset_b = \frac{KT}{q} ln\left(\frac{AR^*T^2}{I_0}\right) \tag{3}$$

The values of ideality factor were calculated by using equation (4)

$$n = \frac{q}{kT}\left(\frac{dV}{dlnI}\right) \tag{4}$$

where $\frac{dV}{dlnI}$ is expressing the value of slope of straight line region of the forward bias and it is extracted from Fig. 1(b). The semi-log plot of ZnO based Schottky diode as a function of temperature can be seen in Fig. 1(c). As the current trasnport mechanism in Schottky diode exhibits the domination of thermionic emission due to linear nature of semi-log plot of I-V at different values of temperature ranging from 300K-1000K. In forward bias due to the presence of resistance in series corresponding to the every value of temperature the direction of current flow in the curvature region is downward.

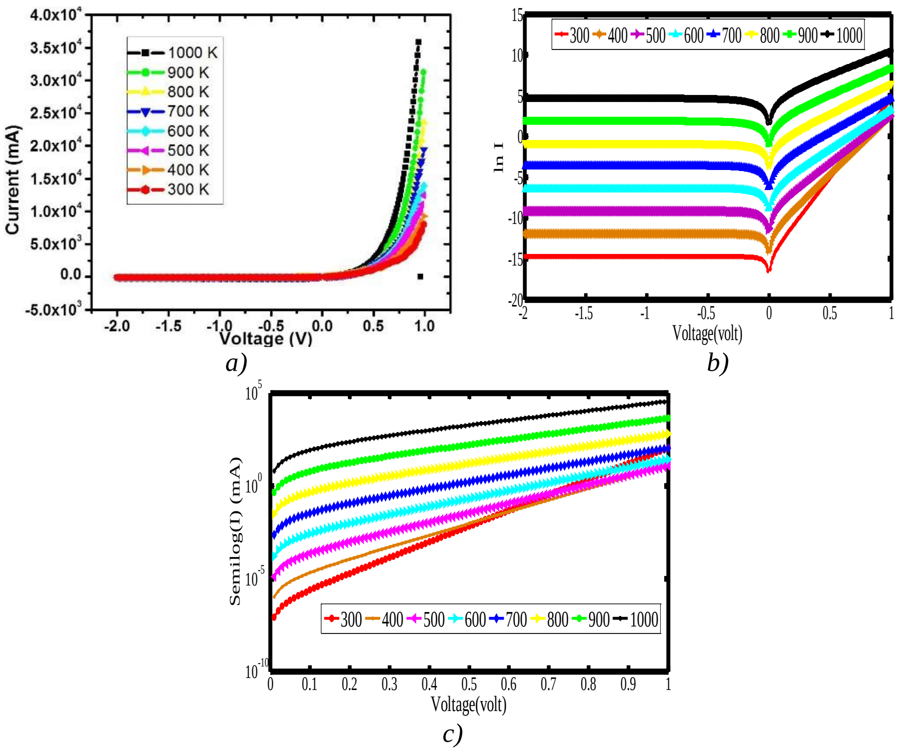

Fig. 1. Current-Voltage characterstics of Schottky diode in the temperature range of 300K-1000K: (a) I-V(b) lnI-V (c) SemilogI-V.

2.2. C.F.

Electrical characteristics of Schottky diode are influenced by a very important parameter which is series resistance . T.E.M. was only used to calculate ideality factor (n) and barrier height (ϕ_b) without considering the effect of series resistance. For non linear and linear region of I-V characterstics, n and ϕ_b are both important parameters but in forward bias I-V characterstics, series resistance is important in downward curvature . Cheung expressed a function to calculate series reistance by I-V characteristics of Schottky diode [37].The following equations from (5) to (7) are associated to the C.F.

$$\frac{dV}{dlnI} = IR_s + \frac{nkT}{q} \tag{5}$$

$$H(I) = V - \frac{nKT}{q}\ln(\frac{I}{AR^*T^2}) \tag{6}$$

$$H(I) = IR_s + n\emptyset_b \tag{7}$$

Here Rs is the series resistance. Using equation (5) $\frac{dV}{dlnI}$ versus I plot was drawn by using data obtained from the downward curvature region of lnI-V plot in the temperature range of 300K -1000K. Fig. 2 is exhibiting the linear relationship between $\frac{dV}{dlnI}$ (V) and I(A). It is in good agreement with published reports . It can be seen that the behaviour in magnitudes of both parameters is same while the temperature is changing. This indicats that the fabricated device will work with consistency. The slope and intercept of equation (5) are showing the values of series resistance and ideality factor respectively.

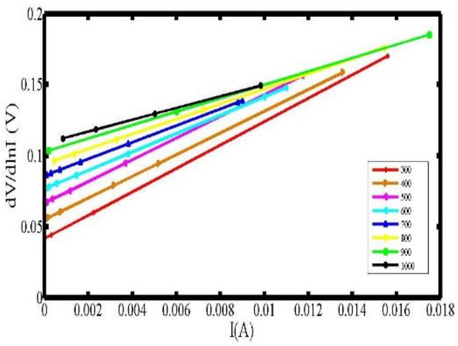

Fig. 2. $\frac{dV}{d\ln I}$ *vs current curve of the ZnO fabricated Schottky diode.*

H(I) versus I plot revealed in Fig. 3 is drawn by using the values of ideality factor calculated from intercept of equation (5). It is indicating that the relationship of C.F. to the current is also linear in this temperature range. No noticeable change except the small linear distance was observed in the temperature variation. The slope and intercept of these straight lines gives series resistance and barrier height respectively against the wide range of temperature from 300K-1000K.

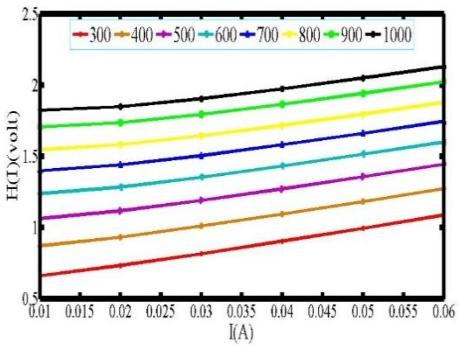

Fig. 3. Cheung function as a function of current I.

3. Comparison among the transportation through T.E.M. and C.F.

The comparison between the calculated values of ideality factor and barrier height obtained by using T.E.M and C.F. is shown in Table 1. All parameters are calculated by using T.E.M and C.F. via MATLAB programing.

Table 1. comparison of calculated values of Schottky diode parameters by using MATLAB.

Temperature (K)	**Thermionic emission model**			**Cheung function**			
				dV/dlnI-I		**H(I)-I**	
	I_s (mA)	**$\emptyset_b$ (eV)**	**n**	**$R_s(\Omega)$**	**n**	**$R_s(\Omega)$**	**$\emptyset_b$(eV)**
300	8.36×10^{-11}	0.85	1.77	8.24	1.61	8.57	0.35
400	1.21×10^{-9}	1.06	1.70	7.65	1.59	8.12	0.48
500	1.74×10^{-8}	1.23	1.62	7.06	1.54	7.73	0.62
600	2.49×10^{-7}	1.36	1.55	6.48	1.48	7.38	0.77
700	3.74×10^{-6}	1.40	1.48	5.89	1.42	7.07	0.92
800	5.48×10^{-5}	1.41	1.41	5.30	1.36	6.79	1.06
900	8.08×10^{-4}	1.60	1.35	4.72	1.32	6.49	1.22
1000	1.21×10^{-3}	1.64	1.29	4.13	1.26	6.28	1.37

Fig. 4 is describing the barrier height of fabricated Schottky diode as a function of temperature. Numerical calculations were performed by using the T.E.M. and C.F. It can be observed from the figure that the calculated values of barrier height via T.E.M were moderately rising with rise in the temperature and the calculated values were in the range of 0.85 eV to 1.64 eV. While the values obtained through the C.F. along with rise of temperature were varying in the range of 0.35 eV to 1.37 eV. All these values are in good agrement with many previouly published reports of experimental work [35,36]. The comparision of both values is revealing the saturation tendancy of barrier heights. A minor difference was found in the comparison, but both have close consistancy with lot of published articles of experimental work [33]. This can be concluded from the obtained results that the barrier height of diodes will increase with the increase in temperature and therefore the performance of the device will be much better due to the less resistance in transportation.

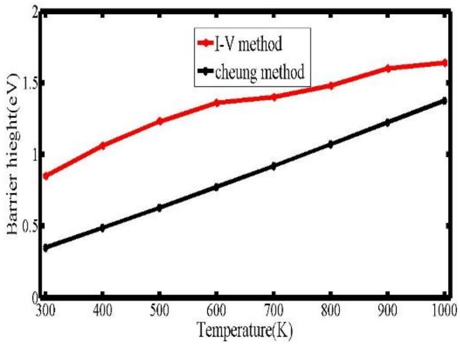

Fig. 4. Barrier height as a function of temperature.

Fig. 5 is expressing the relationship of ideality factor as a function of temperature. The ideality factors were calculated by using the T.E.M. and C.F. The values obtained through both models showed the similar trend from low temperature to high range of temperature. The values of ideality factors were decreasing with rise in temperature and going to be saturated after attaining 1.7 via T.E.M. and 1.6 via C.F. The comparison between the obtained values clearly indicates that ideality factor decreases with increase in temperature. These calculated values also showed good aggrement with many published reports [38].

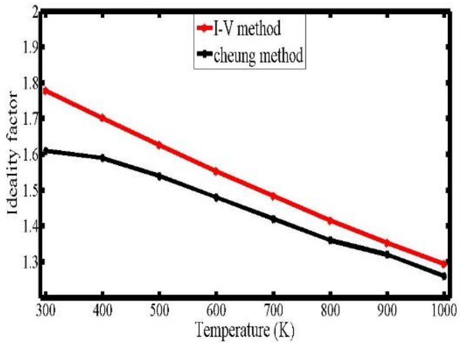

Fig. 5. Ideality factors as a function of temperature.

Fig. 6 is revealing the comparison of series resistance calculated through $\frac{dV}{dlnI}$ -I and H(I)-I graphs as a function of temperature. The obtained values in both cases showed the similar trend from low temperature to high range of temperature. Fig. 6 is clearly showing the similarity in the values of series resistance calculated by equation (5) and(7) and the value of series resistance decreases with increasing temperature.

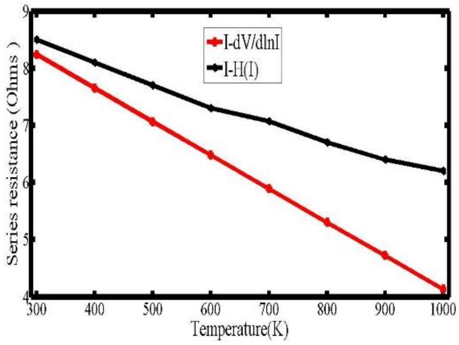

Fig. 6. Series resistance as a function of temperature.

4. Conclusions

This study will not only open the gate for the numerical investigation beyond the temperature range of 673K, but the obtained results proved that instead of doing experimental work at macro level it is better to use numerical simulations to save both time and cost. In the temperature range of 300K–1000K the electrical parameters like barrier height, ideality factor and series resistance of Schottky diode were investigated. The barrier height and ideality factor have been calculated through MATLAB by utilizing thermionic emission model and Cheung function.

Results obtained through both models were compared and it was found that barrier height increases and ideality factor decreases with increase in temperature. More over the I-V characterstics showed strong dependence on temperature. The series resistance was also been calculated by using different equations of Cheung function and it was observed that the value of series resistance decreased with increase in temperature.

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