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SEMICONDUCTOR STRUCTURES, LOW-DIMENSIONAL SYSTEMS, AND QUANTUM PHENOMENA

A New Simulation Model for Inhomogeneous Au/*n*-GaN Structure[1]

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Abstract—The larger the device area, the more difficult to carry on homogeneity during the fabrication and following treatments. Structural inhomogeneity may indicate themselves in variations in local electronic device parameters. Electrical current through the potential barriers is exponentially sensitive to the local device parameters and its fluctuations in the Schottky devices. A new simulation program is developed to describe a relation between multiple, random barrier heights and current-voltage characteristics of the Schottky device. We model the barrier height inhomogeneity in terms of random microcells connected in parallel, which have different barrier height values. Analyzing the integral of the simulated light current-voltage curves show that fluctuations of the local barrier height result in a degradation of the open circuit voltage, fill factor and in consequence, of the over all power conversation efficiency. The implementation described here is quite general and can be used to simulate any device parameter fluctuations in the Schottky devices.

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1. INTRODUCTION

Number of physical problems depend on the inhomogeneity arise from large area thin film device fabrication processes. Numerical modeling of devices is a realistic approximation for exploration of device behaviors. An equivalent circuit model consisting of parallel connected diodes with different electronic quality simulates the electronic properties of the inhomogeneous device. In this study, we examined the effects of the local barrier height variations on the light current voltage (*I*–*V*) characteristics, open circuit voltage, and fill factor. Simulation program has been developed and operated for the Au/*n*-GaN device structure. GaN is a wide bandgap material (3.4 eV) and it is the most promising material for the fabrication of light emitting diodes, lasers, detectors, photovoltaic energy conversation, fiber optic communication, high-temperature, highpower and high-frequency transistors applications due to its direct bandgap [1–3].

Randomly distributed dopand atoms within the semiconductor, atomic steps and lattice defects at the interface, the relative orientation of semiconductor and metal atoms, grain boundaries in the metal, interface roughness bring on laterally varying Schottky barriers [4–12]. Nonuniform interfacial on a semiconductor leads to parallel contacts between metal and semiconductor. Penetration of metal through semiconductor makes localized contacts to semiconductor. Maffeis et al. reports evidence of Au–GaN intermixing regions at Au/GaN interface [13]. Also, they viewed this layer by TEM. This layer consists of Au grains embedded in a GaN matrix. The complex interface brings about the abnormal diodic properties. Understanding the electrical characteristics of these devices naturally induces a number of challenges. Very little is known about the characteristics of devices with parallel contacts and new studies should be conducted to clarify the issue. Direct images of Schottky barrier height fluctuations in the devices have been obtained using ballistic electron emission spectroscopy and researchers correlated them with a Gaussian distribution function. Simulation studies for investigation of the effect of the Gaussian distribution of the barrier heights on the current voltage characteristics had been reported in the literature [14–18].

Computer simulations have become a convenient part of mathematical modeling of many devices for optoelectronic applications. One can analyze, design and operate complex systems by simulation. A simulation model mimics to algorithms and equations used to represent the behavior of the device being modeled. The suitable handling of inhomogeneity effects is necessary both for calculating accurate current voltage characteristics and the study of lateral inhomogeneities with numerical simulations [19, 20]. Numerical modeling and simulation of devices are useful for developing the newer technologies and the low priced methods to test device operations and optimizations. A proper understanding of the device characterization

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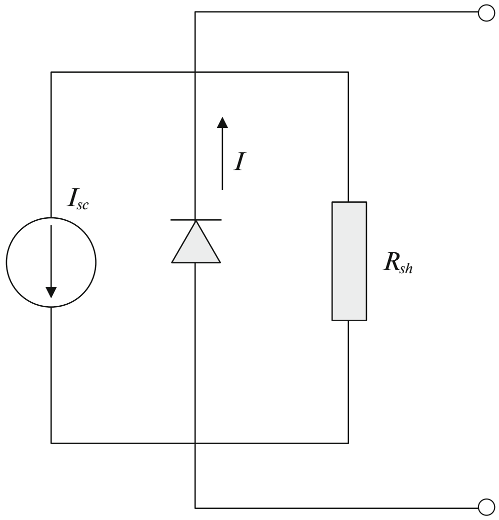

Fig. 1. Equivalent circuit elements consist of a current source I_{sc}, a parallel resistance R_{sh} and a diode with current I. For simulation purposes, the device is divided j microcells. Each microcell represents a discrete circuit unit.

is crucial since it is a powerful tool to calculate the physical and electronic parameters of a device. Modeling enables us to see how a real world performance of the devices will fulfill under different conditions. In the meantime, understanding the nature of inhomogeneity effect on the device performance will be a vital endeavor in the near future for improvement of Au/*n*-GaN devices or other devices.

In this study, the key parameter is the characteristic barrier height fluctuations in the device. Device was assumed to have inhomogeneous barrier height and changes in barrier heights of microcells were considered to be random. Current depends exponentially on the value of the Schottky barrier height. Barrier height fluctuating effect on the I–V characteristics of the Au/*n*-GaN device has been studied by developed simulation software using more general fundamental semiconductor device equations. During the simulation process, Au/*n*-GaN device is interpreted based on the existence of the barrier height inhomogeneities.

2. METHOD OF NUMERICAL SIMULATION

We simulate the current voltage characteristics of inhomogeneous device by connecting different microcells in parallel. The current voltage characteristic of a single element, which is shown in Fig. 1, is represented by Shockley equation [21].

$$I(V) = AA^*T^2\exp\left[-\frac{q\Phi_{bo}}{k_{\mathrm{B}}T}\right]\left[\exp\left(\frac{q}{nk_{\mathrm{B}}T}V\right)-1\right] + \frac{V}{R_{sh}} - I_{sc}, \qquad (1)$$

where A is the diode area, A^* is the effective Richardson constant, T—temperature, Φ_{bo}—barrier height, k_{B}—Boltzmann constant, q—the electron charge, n—the diode factor, R_{sh}—shunt is resistance, I_{sc}—the light generated current.

Actually, inhomogeneities in the device are unavoidable and are present invariably even in the most carefully fabricated system. When modeling different kinds of junctions, a single exponential Shockley equation is not enough to display variations of several electrical parameters in the device. In this study, electronic properties of the inhomogeneous device are simulated by connecting different microcells in parallel, such as one shown in Fig. 1. The system is considered to have a number of non-interacting microcells with each corresponding to a different barrier height within the distribution limit. The current voltage characteristic of a microcell is exponential, because of this microcells can be exponentially sensitive to small variations in the local device parameters. The current is assumed to be a sum of the currents following in all the individual microcells. The simulation studies performed on Au/*n*-GaN device assume one constant series resistance for all microcells.

The barrier height control and distribution in the device is very important in determining the performance of devices such as diodes and transistors. Our main goal is to investigate barrier height inhomogeneity effect on electrical characteristics by developed simulation program. The illuminated current-voltage characteristics for 0.4 × 0.4 cm^2 area of Au/*n*-GaN device are obtained from developed simulation program. Microcells are assumed to be square in shape. The device is sliced into 40 by 40 microcells to cover an area 100 $\mu\mathrm{m}^2$ each. Total cell number in the device is 1600. Each microcell represents a discrete circuit unit under light as seen in Fig. 1. Any deviation of a microcell parameter from the rest of the microcells would indicate inhomogeneity.

Barrier height of each microcell to be different from each other is introduced to program in accordance with the following formula:

$$\Phi_{bo,j} = \phi_{bo}(0) + (\Gamma\phi_{b0}(0))(2RND - 1), \qquad (2)$$

where j is the cell number, $\phi_{b0}(0)$ is the zero bias barrier height offset value, Γ is the barrier height fluctuation factor, *RND* is the random generated number varies between 0 and 1. The distribution pattern of barrier height is characterized by Γ, which is percentage deviation from the zero bias barrier height offset value. $\phi_{b0}(0)$ value is introduced from experimental studies [22]. Random distribution of zero barrier height in the device is shown in Fig. 2. Gamma (Γ) is a measure of inhomogeneity. Inhomogeneity is introduced to program via fluctuation factor term whereby barrier height of each microcell is different from each other's represents inhomogeneity. Barrier height variation from first cell to final cell in the device has been successfully used for inhomogeneous device modeling.

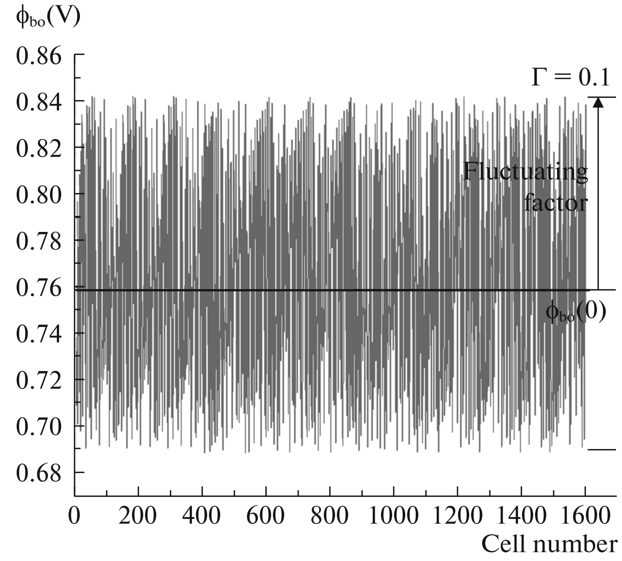

Fig. 2. Fluctuation of barrier height around a constant value from first cell to final cell.

During the studies, other than the barrier height of the device parameters were kept constant.

Our developed simulation program runs as given below lines:

Input endpoints $V_{\min}$, $V_{\max}$ and positive integer n (number of data).

Input cell number.

Step 1: Input the offset value ($\Phi_{bo}(0)$).

Step 2: Input the fluctuating factor of barrier height.

Step 3: Barrier height values of each microcell were fluctuated around constant value according to Eq. (2) for $j = 1$ to cell number. Perform the simulation and barrier height values for each microcell.

Step 4: Next j.

Step 5: For $V = V_{\min}$ to $V_{\max}$ step dV.

Step 6: For $i = 1$ to cell number do step 7.

Step 7: The total current through the device is calculating by simply adding the individual current through each microcell using electronic device parameters:

$$I = \sum_{j=1}^{\text{cell number}} \left(AA^* T^2 \exp\left[\frac{-q\Phi_{b0j}}{k_B T}\right] \times \left[\exp\left(\frac{q}{n_j k_B T}(V - IR_s)\right) - 1\right] + \frac{V - IR_s}{R_{sh\,j}} - I_{sc\,j} \right).$$

Step 8: Next i.

Step 9: Next V, where R_s is the series resistance.

The suggestion is that there are a number of parallel microcells of different barrier heights, each contributing the current individually. The device is modeled in the presence of a parasitic resistance for all microcells and individual shunt resistances of microcells by the summation of multi exponential expressions, plus resistive shunt terms and minus light generated current terms. We have evaluated simulation program to investigate dependence of I–V characteristics on barrier height fluctuations in the device. Simulation data presented in this study deals with AM0 solar spectrum and at room temperature.

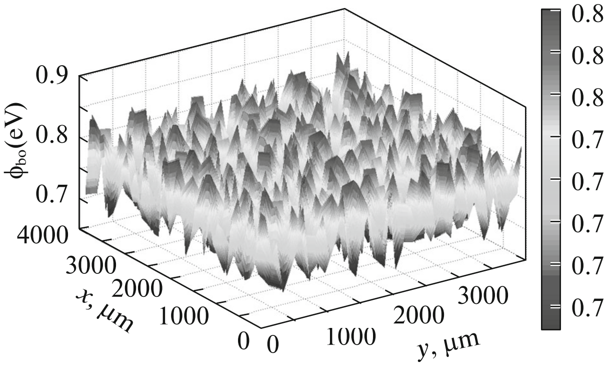

Fig. 3. An example of randomized fluctuations in the barrier height of the Au/n-GaN device. In this case fluctuation factor is 0.1.

3. RESULTS AND DISCUSSION

In this study, rigorous numerical calculation of illuminated current voltage characteristics were carried out by using a simulation program developed by our group for an Au/n-GaN device structure. The system is considered to have a number of non-interacting parallel microcells with each corresponding to a different, random barrier height within the distribution limit.

1600 regions of increasing or decreasing barrier height enforce alternations in the barrier height in the Au/n-GaN device. Barrier height values are randomized around the barrier height offset value. The randomness of the barrier height values has been tested with chisquare test.

The magnitude of the barrier height is determined by fluctuation factor.

Inhomogeneities in the device can be characterized in terms of the local values of the barrier height. Figure 3 shows an example of the local barrier height variation in the Au/n-GaN device.

Current voltage characteristics of the Au/n-GaN device are simulated for room temperature and different barrier height fluctuating factor values. Figure 4 represents the illuminated current voltage characteristics of the Au/n-GaN device. It is quite clear that the illuminated current voltage characteristics are sensitive to the barrier height fluctuating factor.

One of the difficulties for the improvement of efficiency in optoelectronic devices is relatively low V_{oc} (open circuit voltage). Figure 4 shows barrier height fluctuating factor dependent illuminated current voltage characteristics of Au/n-GaN device. The barrier

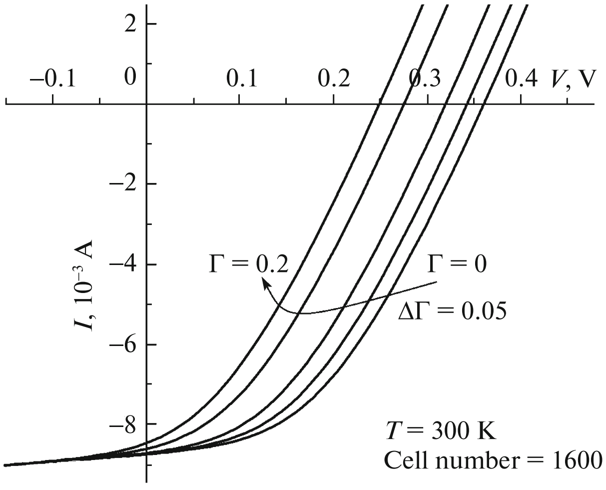

Fig. 4. The illuminated current voltage characteristics of the multi diode simulations for variations in the barrier height.

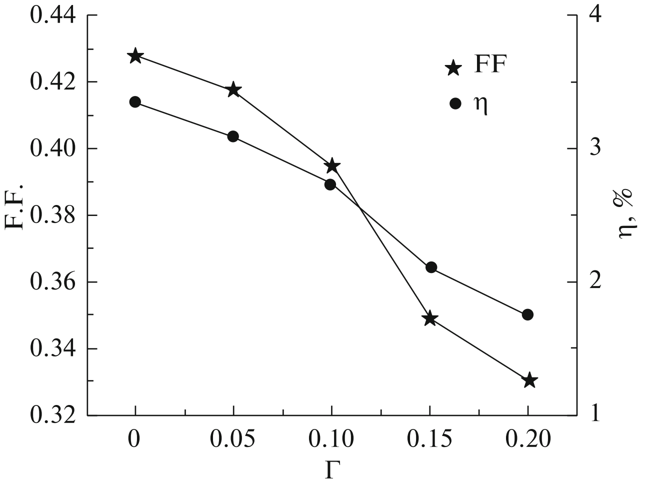

Fig. 5. Barrier height fluctuating factor dependent fill factor (FF) and efficieny (η).

height fluctuating factor primarily affects to the V_{oc}. Simulation results clearly display that when the inhomogeinity increases V_{oc} decreases as reported by Malm et al. [23].

With the help of one diode model equation under light (with $R_s = 0$ and $R_{sh} = \infty$ and neglecting the one in the diode law), it is obtained Eq. (3) for homogeny device [21]:

$$V_{oc}^{0} = \frac{E_g}{q} - \frac{k_{\mathrm{B}}T}{q}\log\left(\frac{AA^{*}T^{2}}{I_{sc}}\right). \tag{3}$$

If there is inhomogeneities in the device, Eq. (3) is represented as Eq. (4):

$$V_{oc} = V_{oc}^{0} - \ni, \tag{4}$$

where V_{oc} and V_{oc}^{0} are the open circuit voltage of inhomogeneous and homogeneous device, respectively; $\ni$ term stems from inhomogeneities in the device.

The reverse saturation current is given by:

$$I_0 = AA^{*}T^{2}\exp\left(-\frac{q\Phi_{bo}}{k_{\mathrm{B}}T}\right). \tag{5}$$

$\Phi_{bo} \approx 2E_g/3$ is for the depletion contact formed on *n*-type substrate (E_g is the band gap energy). Consequently, fluctuations of barrier height means band gap inhomogeneity in the device hence result in $\ni$ in Eq. (4). Band gap of the materials is affected by growth techniques. Band gap engineering is the process of controlling or altering the band gap of a material by controlling the composition of certain semiconductor alloys. The motivation for the materials growths is to produce suitable band gap materials for use in optoelectronics. Precise control of the composition, thickness, uniformity and doping levels is investigated [24].

Several simulation studies have been performed with changing the fluctuation factor values. Our simulation studies show that barrier height fluctuation factor values are very important in optimization of optoelectronic device fill factor and efficiency values. A decrease has been seen in the fill factor and the efficiency, with the increasing of barrier height fluctuating factor.

Fluctuations in the barrier height of disordered microstructures due to spatial fluctuations in the microstructure of the device strongly affect current voltage characteristics. For handling optimum device performance, device layers to be uniform in composition with any fluctuations in barrier height must keep to a minimum. It is seen that V_{oc} value of the device is strongly governed by barrier height fluctuating factor.

The barrier height fluctuating factor also affects fill factor, and hence the power loss. Several optoelectronic device materials are prepared by different techniques. Some of them have gathered much attention as new age device material by reason of simple fabrication process, mass produceability and material economization. Recently, researchers show that high efficient optoelectronic devices can be achieved by fabricating homogeny device structures. Reports display that key technology to obtain especially high V_{oc} and fill factor is the grain size and electrically homogeneous structures. Barrier height fluctuating affects inversely efficiency and fill factor of the device as seen in Fig. 5.

4. CONCLUSION

Device modeling of Au/*n*-GaN device has been investigated with taking barrier height fluctuating factor into account by simulation. It has been found that barrier height fluctuating factor is of importance for enhancing V_{oc}, efficiency and fill factor. Developed simulation program offers a favorable tool not only for optimum design, but also performance analysis of optoelectronic devices.

It is displayed that a strong correlation between barrier height fluctuating factor and illuminated current voltage characteristics of Au/*n*-GaN device. Fluctuating factor values have been found to be responsible for the current transport across the Au/*n*-GaN device with spatial inhomogeneity. As the simulation results of Au/*n*-GaN device show, V_{oc}, fill factor, and efficiency considerably follow the barrier height fluctuating factor. The barrier height fluctuation factor is an important parameter that strongly affects the device characteristics, which should be taken into account in the realistic simulations. We believe that understanding effects of barrier height inhomogeneity will help to improve device performance and stability.

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