Intersection behavior of the current–voltage (I – V) characteristics of the (Au/Ni)/HfAlO₃/n-Si (MIS) structure depends on the lighting intensity

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Abstract

The current–voltage (I – V) and capacitance–voltage (C – V) behaviors of the (Au/Ni)/HfAlO₃/n-Si (MIS) junctions at room temperature under white light with various intensities were investigated. The $\ln(I)$ – V curves show two linear behavior regions at about 1 V before and after the point of intersection that can be defined as two separate current-conduction (CMs) Mechanisms. The values of the ideality factor (n) and the zero-bias barrier height (Φ_{B0}) were extracted using the slope and intercept of the $\ln(I)$ – V curve before and after the intersection point based on lighting power. Although the Φ_{B0} values decrease with increasing light power, n increases for two regions, and there is a strong linear relationship between them. The values of photo-current (I_{ph}) increase with the increasing lighting power due to the formation of electron–hole pairs. The slope of the double-logarithmic I_{ph} – P was changed from 0.422 to 0.852, respectively, at -2 V and -9 V, which indicates the ongoing distribution of N_{ss} . In addition, the profile of surface states (N_{ss}) ionized by light was obtained from the capacitance measured in dark and under lighting at 1 MHz. The N_{ss} – V curve has two characteristic peaks that correspond to the region of depletion and accumulation due to a special distribution of N_{ss} and their restructuring and reordering under the effects of lighting and an electric field.

1 Introduction

The metal–semiconductors (MS) and metal–insulator–semiconductors (MIS) structures have long been a trendy technology, such as integrated circuit diodes, MIS capacitors, photodiodes, and other applications. Especially the MIS photo-diode and photo-detector experiments have been getting deeper and broader in recent years [1–3]. The manufacturing processes and the creation of an interface layer

between the metal and a semiconductor play significant roles in the performance of this structure, its barrier heights (BH), and conduction mechanisms (CMs) [4–6]. The reaction of the Schottky structure to the applied bias voltage, temperature, frequency, and intensity of light has a direct effect on certain optoelectronic devices. The performance of MS and MIS devices can be optimized by various factors, such as the choice of metal and semiconductor with acceptable work functions, appropriate doping (donor/acceptor atoms) level, interface layer, and its homogeneity and thickness, low density of N_{ss} , low series resistance (R_s), and homogeneity of BH [7, 8]. Furthermore, the optical behavior and photo-response of a diode can be improved by changing the interface layer. The photo-current was stated to have low-voltage saturation characteristics due to the limitation of the minority carrier. Because *high-k* materials play an important role in the efficiency of MIS structures, many researchers tried to prepare MIS devices with *high-k* thin films as the insulator layer to reduce saturation at low voltage [9, 10].

The HfO₂ has drawn significant interest for both resistive oxide and optical materials thanks to its strong thermal and chemical stability [11], high dielectric constant (~ 25) [12], and wide bandgap (5.8 eV) [13], and has a good

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transmittance especially in ultraviolet light [14]. Depending on the above-mentioned properties, the basic HfO_2 has a vast range of applications involving resistive switching [15], UV anti-reflective film, and gate dielectrics in the Schottky structures [16–18]. However, there is a significant disadvantage for this substance, which is its poor thermal stability and the comparatively low crystallization temperature (400–450 °C) [16]. These properties cause a significant increase in the leakage current if HfO_2 films are incorporated in a high-temperature MIS system. To increase the crystallization temperature and enhance the electrical properties of HfO_2 , it can be converted to alloy HfAlO_x (hafnium aluminum) using aluminum oxide (Al_2O_3) intermixed [19–21]. Furthermore, the integration of the Al into HfO_2 causes an increase in its dielectric constant and bandgap as well as decreases its hysteresis and charging defects. All of these properties of HfAlO_x make it an excellent material for use in MIS systems of future technology as an alternative to other dielectric materials.

The conduction mechanism of MS and MIS Schottky structures under the light can be quite different from those in the dark. These structures with oxide interface layers sometimes show a photo-response behavior [14, 18]. For this reason, current–voltage (I – V) measurements of such structures under different lighting intensities can give us important information about the basic current-conduction parameters such as CMs, BH, and performance of the structure. [22, 23]. Generally, the capacitance values of an MIS structure and also the basic electrical parameters such as ideality factor (n), BH (Φ_{B0}), series and shunt resistances (R_s and R_{sh}), and the density of interface states (N_{ss}) can be strongly influenced by lighting intensity [24]. On the other hand, there are various theoretical and experimental studies investigating the point of intersection in the I – V graph of the MIS structure calculated at various temperatures. These studies have explained that the intersection point can occur due to the decrease in apparent barrier height with decreasing temperature and the presence of R_s [25–27].

There are several studies on the dielectric characteristics of the HfAlO_x alloys, but none of the studies focus on their photo-diode characteristics or their reaction to light as MIS structures, while the investigation of optical behavior plays a significant role in such studies and implementations of alloys. Therefore, it is important to investigate the light power-dependent electrical and optical characteristics. The present paper explores the key electrical parameters of (Au/Ni)/ HfAlO_3 /n-Si MIS structure such as n , BH, and R_s based on the white light intensity. For this, both the forward and reverse bias I – V characteristics of this device were done at the light power range of 0–300 W. The experimental results show that the $\ln(I)$ – V curves display two linear sections that can be represented as two separate CMs before and after an intersection point. Furthermore, the voltage-dependent

capacitance behavior was measured in dark and under the illumination of 300 W light and the N_{ss} was obtained from the measured capacitance values in dark and under illumination.

2 Experimental procedures

The phosphor-doped silicon wafer (n-Si) with $\langle 100 \rangle$ float zone, $\sim 300 \mu\text{m}$ thickness, and $1 \Omega \text{ cm}$ resistivity was cleaned using RCA-1 and RCA-2 standard cleaning procedures to remove the metal ions, a thin oxide layer, and organic residues of the wafer surface. The cleaned wafer was then moved to the thermal evaporation system and Al metal (99.999%) with a thickness of 300 nm was formed on the backside of n-Si at $\sim 1 \times 10^{-5}$ Pa. The formation of an Ohmic contact was then annealed at 450 °C for 20 s in N_2 ambient. The production of devices continued with the growth of 80 nm ternary HfAlO_3 alloys on the substrate using Cambridge Nanotech. Inc. Savannah/S100 Atomic Layer Deposition (ALD) system. Deposition of 300 Cycles led to 80 nm of thin HfAlO_3 film. H_2O , $\text{Al}(\text{CH}_3)_3$, H_2O , and $\text{Hf}(\text{NMe}_2)_4$ are used as precursors and are successively added into the chamber to complete a cycle. In each cycle, the pulse and purge times are 0.015 s and 8 s, 0.015 s and 8 s, 0.015 s and 10 s, and 0.2 s and 15 s, respectively, for each precursor.

The atomic ratios of the hafnium (Hf), aluminum (Al), and oxygen (O) atoms in the HfAlO_3 layer on n-Si substrate were calculated using X-ray Photoelectron Spectroscopy (XPS) quantitative analysis. The thickness-dependent XPS profile of HfAlO_3 layer confirmed that the average atomic fractions are 19.2%, 21.9%, and 58.9% for Hf, Al, and O, respectively; therefore, the atomic ratios of the HfAlO film are very similar to 1:1:3. The thickness of the HfAlO_3 layers was confirmed using a cross-sectional scanning electron microscope (SEM) images as nominally 80 nm.

Using the thermal evaporation method at $\sim 1 \times 10^{-5}$ Pa, the Ni(50 nm)/Au(200 nm) circular rectifier contacts with a 0.005 cm^2 area were finally created on the HfAlO_3 surface. Therefore, the fabrication of an (Au/Ni)/ HfAlO_3 /n-Si MIS structure was completed. The current–voltage (I – V) and capacitance–voltage (C – V) characteristics of the device are carried out using the source-meter Keithley-2400 and the impedance-meter HP 4192A LF, respectively, under the lightning of 0 and 300 W intensity range at room temperature.

3 Experimental results and discussions

Figure 1 shows the measured $\ln(I)$ – V curves of the (Au/Ni)/ HfAlO_3 /n-Si structure in the broad light power range (0–300 W by 50 W steps) and voltage from -9 to $+9$ V by

Fig. 1 The measured $\ln(I)$ – V curves of the (Au/Ni)/HfAlO₃/n-Si structure under lighting with various light intensities. The measured $\ln(I)$ – V curves in dark and the focused graph of the $\ln(I)$ – V curves between 0.3 and 2.0 V under lighting are shown in the insets (a) and (b), respectively

0.05 V steps at room temperature. As depicted in the inset of Fig. 1, the $\ln(I)$ – V curves have an interesting feature in the forward bias region that has almost the common voltage point at nearly 1 V. At this point, the current values are free from the influence of light power. Many experimental and theoretical studies have also reported similar behavior based on temperature or lighting [26–28]. According to Chand [25], the intersection can occur at the same point, but the $\ln(I)$ – V curves are bent for each basic barrier due to the current saturation effect of series resistance. For large structure diameter, this intersection point is shifted to a higher voltage region. Therefore, if we want to observe the intersection of I – V curves, we must reduce the structure diameter to a nanometer scale [27]. These observations in the intersection point of the forward bias $\ln(I)$ – V curves tend to be an unusual behavior compared to the ideal diode in the MS or MIS structure. With an increasing light power, the value of forwarding current decreases after the intersection point due to the lack of free carriers in both dark and low light power conditions. Therefore, although the value of R_s decreases before the intersection point with increasing light intensity, it increases with increasing light intensity after the intersection. This behavior is very unexpected in the nature of Schottky junctions and at first look, it is in contrast with the thermionic emission (TE) concept of the current-conduction mechanisms (CCMs).

According to the theory of thermionic emission (TE), the amount of current passing through the MS or MIS structure at a forward bias ($V \geq 3kT/q$) is presented by [4–6]

$$I = AA^*T^2 \exp\left(-\frac{q}{kT}\Phi_{B0}\right) \left[\exp\left(\frac{q(V - IR_s)}{nkT}\right) - 1 \right] \quad (1)$$

In Eq. 1, the reverse bias saturation current (I_0) is the expression terms in front of the brackets; the IR_s is voltage decrease over R_s ; A^* is the numerical value of Richardson constant ($= 112 \text{ A cm}^{-2} \text{ K}^{-2}$ for n-Si), and T is the temperature in Kelvin. Thus, for each lighting power, the value of n and Φ_{B0} of the (Au/Ni)/HfAlO₃/n-Si structure was determined from the slope and intercept of the $\ln(I)$ – V curves, respectively, as follows [4–6]:

$$n = \frac{q}{kT} \left[\frac{dV}{d(\ln I)} \right] \quad (2)$$

$$\Phi_{B0} = \frac{kT}{q} \ln \left(\frac{AA^*T^2}{I_0} \right) \quad (3)$$

The experimental values of n and Φ_{B0} were acquired from Fig. 2a, b and they changed from 9.915 to 20.924 and 0.732 to 0.672 eV before the intersection point (between 0.30 and 0.7 V) and 15.882 to 23.637 and 0.692 to 0.676 eV after the intersection point (between 1.5 and 2.0 V), respectively. Table 1 summarizes the values of I_0 , n , Φ_{B0} , and R_s derived from Ohm's law ($R_s = V/I$). As can be seen in Table 1 and Fig. 3, while the value of Φ_{B0} decreases with increasing lighting power, n increases and there is a good linear relation between them before and after the intersection point that can be described by two different CCMs.

The higher values of n both in dark and under lighting refer to the presence of N_{ss} , interface HfAlO₃ layer, the Gaussian distribution of BH (Fig. 4) at M/S interface, tunneling current via dislocations in Schottky structures, and generation recombination [5, 6].

All of these findings demonstrate that the HfAlO₃ interfacial layer leads to enhanced light sensitivity as several electron–hole pairs can be produced near the junction under lighting. As seen in Figs. 1 and 5, the photo-current (I_{ph}) values increase with increased lighting particularly in the reverse bias region due to a strong electric field. Recombining electron–hole pairs can obstruct the reverse bias region under a high electric field, but they can easily recombine in the forward bias region due to a low electric field value.

Typically, the photo-current or photo-response attitude of the solar cells or photodiodes can be described with the expression below [27, 29]:

$$\ln(I_{ph}) = m \ln(P) + A \quad (4)$$

here, I_{ph} is the photo-current, A is a constant, P is the power of lighting, and m is an exponent of lighting power. Figure 5 displays the $\ln(I_{ph})$ – $\ln(P)$ curves and the magnitude m was

Fig. 2 The focused $\ln(I)$ - V curves of the (Au/Ni)/HfAlO₃/n-Si structure measured under lighting with various light power, **a** before and **b** after the intersection point

Table 1 Lighting based upon the electrical parameters of the (Au/Ni)/HfAlO₃/n-Si structure

	Before intersection point				After intersection point			
	I_0 (A)	n	Φ_{B0} (eV)	R_s (Ω) (at 0.5 V)	I_0 (A)	n	Φ_{B0} (eV)	R_s (Ω) (at 3 V)
0 W	4.29×10^{-9}	5.57	0.779	2.90×10^7	—	—	—	3.85×10^6
50 W	2.66×10^{-8}	9.91	0.731	2.63×10^6	1.23×10^{-7}	15.88	0.692	6.60×10^4
100 W	5.36×10^{-8}	12.26	0.713	1.89×10^6	1.30×10^{-7}	16.82	0.690	6.90×10^4
150 W	8.47×10^{-8}	14.11	0.702	1.46×10^6	1.37×10^{-7}	17.72	0.689	7.38×10^4
200 W	1.26×10^{-7}	16.31	0.691	1.18×10^6	1.43×10^{-7}	18.95	0.688	8.53×10^4
250 W	1.85×10^{-7}	19.04	0.681	9.45×10^5	1.66×10^{-7}	21.30	0.684	1.10×10^5
300 W	2.71×10^{-7}	20.92	0.671	7.07×10^5	2.27×10^{-7}	23.63	0.676	1.22×10^5

Fig. 3 The Φ_{B0} - n curves of the (Au/Ni)/HfAlO₃/n-Si structure before and after the intersection point

derived from their slope as 0.42 at -2 V and 0.85 at -9 V. These m values suggest the presence of N_{ss} with energies in forbidden bandgap between HfAlO₃ interlayer and n-Si.

Fig. 4 The Gaussian distribution model of BH for Schottky structures

Figure 6 shows the voltage-dependent capacitance (C - V) curves of the (Au/Ni)/HfAlO₃/n-Si structure in dark and under 300 W lighting at a frequency of 1 MHz measured voltage values between -9 and $+9$ V. It is clear that the value of C is considerably increased under light and shows two peaks in the inversion (between -5

Fig. 5 The $\ln(I_{ph})$ – $\ln(P)$ curves of the (Au/Ni)/HfAlO₃/n-Si structure

Fig. 6 The C – V curves of the (Au/Ni)/HfAlO₃/n-Si structure in dark and under the light at a power of 300 W at 1 MHz

and 1 V) and accumulation (between 1 and 9 V) regions. The observed two distinctive peaks with light effect in the C – V (Fig. 6) curve are the result of a special density distribution of N_{ss} due to their restructuring and reordering. While the first peak is corresponding to the inversion region, the second peak is corresponding to the accumulation region. Therefore, the lighting-induced values of N_{ss} were acquired from the dark-lighting capacitance method ($C_d - C_i$) by using the following expression and are given in Fig. 7 [22].

Fig. 7 The voltage-dependent profile of N_{ss} for (Au/Ni)/HfAlO₃/n-Si structure

$$qAN_{ss} = \left[\left(\frac{1}{C_d} - \frac{1}{C_i} \right)^{-1} - \left(\frac{1}{C_l} - \frac{1}{C_i} \right)^{-1} \right]. \quad (5)$$

As seen in Fig. 7, the voltage-dependent surface states' profile (N_{ss} – V) has two distinctive peaks like C – V curve. This is evidence of the existence of localized surface states with two different regions and life times. These surface states are induced under an external force such as electric field, temperature, or light and they act as recombination centers that can be release or capture electronic charges. Therefore, in this work the lighting causes an increase in the capacitance value. The observed first peak in the C – V curve in the inversion region is only the result of surface states at HfAlO₃/n-Si interface. However, the second peak in the accumulation region is the result of both series resistance and surface states. These results show that the surface states in the inversion region are more effective than that in the accumulation region. Similar two peaks' behaviors in the C – V curve under radiation are also observed in the literature [30, 31].

4 Conclusion

In this study, both the forward and reverse bias I – V and C – V characteristics of the fabricated (Au/Ni)/HfAlO₃/n-Si (MIS) structures were investigated in the dark and under lighting in a wide voltage range (± 9 V) and at room temperature. The semi-logarithmic I – V curves for various lighting power have two linear parts before and after an intersection point at about 1 V. Such an interesting feature of these curves shows the existence of two different mechanisms of current

transport. The obtained experimental values of n and Φ_{B0} using the slope and intercept of $\ln(I)$ – V curves are found to be a strong function of lighting intensity both before and after the intersection point regions. The values of Φ_{B0} decrease with increasing lighting intensity, whereas the n values increase for two regions. The observed increase in I_{ph} with lighting is the result of electron–hole pair generation and obey the power-law ($I_{ph} = AP^m$). Therefore, the value of m was found as 0.422 for -2 V and 0.852 for -9 V. These values of m indicate the presence of the continuous distribution of N_{ss} between the $HfAlO_3$ interface layer and n -Si. The voltage density distribution of the N_{ss} profile was also obtained from the measured C – V values in dark and under lighting at a frequency of 1 MHz. The N_{ss} – V curve has two broad peaks located in the depletion and accumulation regions due to a particular density distribution of N_{ss} and their restructuring and reordering under lighting and an electric field.

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