ILLUMINATION DEPENDENT ELECTRICAL CHARACTERISTICS OF PTSi/n-Si(111) SCHOTTKY BARRIER DIODES (SBDS) AT ROOM TEMPERATURE

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Abstract. The electrical characteristics of PtSi/n-Si (111) Schottky barrier diodes (SBDs) with diffusion barrier have been investigated by using the current-voltage (I-V), capacitance-voltage (C-V) and conductance-voltage (G/ω-V) measurements both in dark and under various illumination intensities. The revealing of main parameters such as barrier height (Φ_B0), ideality factor (n), the depletion layer width (W_D), the distribution of doping concentration atoms (N_D) were found a function of illumination intensities. The peak behavior of series resistance (R_s) of the diode is practically independent of illumination level. The reverse bias of C-V plot exhibits two linear regimes with different slopes which are corresponding (0.2-0.4)V and (0.6-0.8) V and revealed the presence of two barriers for all illumination levels for PtSi/n-Si(111) SBD. We have attributed this behavior to increasing of doping degree due to process of formation of silicide/silicium contact and crystal structure of Si(111).

Keywords: PtSi/n-Si SBDs, I-V, C-V and G/ω-V measurements, diffusion barrier, Illumination effect on electrical parameters, inhomogenity interface, two barriers.

1. Introduction

Metal-semiconductor (MS) contacts with and without interfacial layer usually are known Schottky barrier diodes (SBDs) and they are more important both in electronic and optoelectronic applications. Recently, the formation of silicide compounds at metal/Si (M/S) interface becomes more popular in the applications to need for basic understanding of the properties of M/S interface. The performance, quality and reliability of Schottky diodes are dependent various parameters such as the formation of interface processes, charges localized at M/S interface, doping concentration, crystal structure, series resistance of diode, interfacial layer, temperature and illumination. Especially, the formation of silicide compounds at metal/Si (M/S) interface influences on electro-physical parameters of diodes [6, 12, 19, 22, 24, 25, 27, 32, 33]. Metal silicide/silicon contacts including PtSi/Si have been subject of both experimental and theoretical studies in the past decades [10-13, 15-17, 19, 20, 22, 32, 33]. Yet, the illumination effects and influence of crystal structure of contacting materials on the main electrical parameters of /Si structures have not yet been investigated in detail. In
addition, this SBDs were fabricated with diffusion barrier (amorphous alloy TiW) to prevent diffusion of Al, traditionally used as ohmic and rectifier contact. The aim of this study is to investigate the effect of illumination on the main electrical parameters of PtSi/n-Si(111) SBD with diffusion barrier under various illumination intensities in the wide range of applied bias voltage at room temperature by using I-V, C-V and G/ω-V measurements.

2. Experimental Procedures

The PtSi/n-Si (111) SBDs were fabricated on the 3inc diameter n-type (P-doped) single crystal silicon wafer with (111) surface orientation, 0.7 Ω cm resistivity and 3.5 μm thickness. For the fabrication of PtSi/n-Si (111) SBDs have been used the methods of planar technology, standard photolithography and magnetron sputtering [1-3]. To prevent diffusion of Al amorphous alloy TiW has been used as diffusion barrier between PtSi and Al. All processes were carried out in room with 100 class. Thus, the produced chip contains 14 diodes with different areas (1x10^-6-14x10^-6 cm^2) were completed and both the structure of the fabricated chip and cross section of PtSi/n-Si (111) SBDs were given in Fig. 1(a) and (b) respectively. In this study, only the results of diode with the area of 8x10^-6 cm^2 are presented.

The current-voltage (I-V) measurements were performed by the use of a Keitlley 220 programmable constant current source and a Keitlley 614 electrometer at room temperature. The C-V and G/ω-V measurements of the fabricated PtSi/n-Si(111) SBDs were performed by the use of an HP 4192 A LF impedance analyzer (5 Hz-13 MHz).

All measurements were carried out with the help of a microcomputer through an IEEE-488 AC/DC converter card. For the illumination of sample, a 250 W solar simulator (Model: 69931, Newport-Oriel Instruments, Stratford, CT, USA) was used as a light source. The photons at different power levels were passed through an AM1.5 filter which allowed wavelengths only between 400 and 700 nm to be incident upon the diodes. The intensity of the light was measured by research radiometer (Model ILT1700, International Light Technologies, Massachusetts, USA). Illumination dependent measurements were carried out under 10, 25, 40, 63, 80, 100 mW/cm^2 illumination levels.

3. Results and discussion

The forward and reverse bias I-V characteristics of the PtSi/n-Si (111) SBDs were measured at room temperature both in dark and under various illumination intensities in the voltage ranges of (-25 V)-(+5 V) by 50 mV steps at room temperature and they were given in Fig. 2. While the forward bias InI-V characteristics of the diode are almost independent on illumination level, but the reverse bias InI-V characteristics were found a strong function of due to high electric field in the junction.

As shown in Fig.2, InI-V plots both in dark and under 100 mW/cm^2 are linear in the voltage range of 0.075 V-0.5 V, but they deviated considerably from
the linearity especially due to the effect of $R_s$ and native interfacial layer for adequate high forward bias voltages ($\geq 0.5$ V). When bias is across on the diode, it will be shared by $R_s$, native interfacial layer and depletion layer of the structure. The “soft” breakdown behavior observed as a function of bias in the experimental reverse bias branch in Fig. 2 may be explained in terms of spatial inhomogeneity of barrier height (BH) and image force lowering [8, 26].

It is clear that the change in illumination level has important effects on the determination of the main diode parameters such as $\Phi_{Bo}$, n, $I_o$. For MS type SBDs with and without interfacial layer with $R_s$ when n is higher than unity, the relationship between I and V in terms of thermionic emission (TE) theory ($V \geq 3kT/q$) is given as [6, 24, 25, 27]:

$$I = I_o \left[ \exp\left(\frac{q(V - IR_s)}{nkT}\right) - 1 \right]$$

(1)

Here $V$ is applied forward bias voltage across the diode, $q$ is the electronic charge, $k$ is the Boltzmann constant, $T$ is the absolute temperature in Kelvin, the term $IR_s$ is voltage drop across $R_s$ and $I_o$ is the reverse-saturation current which is given by:

$$I_o = AA^*T^2 \exp\left(\frac{-q}{kT}\Phi_{Bo}\right)$$

(2)

where $A$ is the rectifier contact area, $A^*$ is the effective Richardson constant that equals 264 A/cm$^2$ K$^2$ for (111) orientation n-type Si [1-4], $\Phi_{Bo}$ is the zero-bias BH. The value of $I_o$ can be obtained by extrapolating the linear portion of the lnI-V plot to the intercept point with the current axis at zero applied voltage at each illumination levels. Thus the value of $\Phi_{Bo}$ can be extracted from Eq. 2 as following relation for each illumination level:

$$\Phi_{Bo} = \frac{kT}{q} \ln\left(\frac{AA^*T^2}{I_s}\right)$$

(3)

The values of n and $I_o$ were found as 1.22 and 2x10$^{-10}$ A in dark, 1.57 and 1x10$^{-9}$ A under 100 mW/cm$^2$, respectively. The values of $\Phi_{Bo}$ were calculated from Eq. (3) as 0.71 eV and 0.67 eV for in dark and under 100 mW/cm$^2$, respectively. As shown, the main value of the electrical parameters of the structure such as $\Phi_{Bo}$, n, $I_o$ are considerably dependent of illumination.

The capacitance-voltage (C-V) measurement is a widely used method to get more information on electrical characteristics of the MS type SBDs[3],[4]. The illumination dependent C-V and G/ω-V characteristics of PtSi/n-Si(111) SBD are measured both in dark and under various illumination levels (10, 25, 40, 63, 80, 100 mW/cm$^2$) and given in Fig. 3 (a) and (b), respectively. These measurements were performed at enough high frequencies (500 kHz) with a small ac signal of 40 mV peak to peak amplitude at room temperature in voltage range of (-4 V)-(+ 6 V) by 50 mV steps. As can be seen from these figures, both the values of C and G/ω increase with increasing illumination level and these changes in C and G/ω with illumination are quite high in depletion and accumulation region values vary from (-4 V) to (6 V).

On the other hand, these changes in C and G/ω values remain almost constant in the inversion region. The high values of C and G/ω under high level
illumination intensity can be attributed to the excess capacitance and conductance resulting from the illumination induced electron-hole pairs. The value of C starts a sharp increase in forward bias (V≥0.7V) when the illumination intensity increases, but it has a concave curvature in the strong accumulation region due to the effect of $R_s$. The maximum value of the C and its position may be depended on various parameters such as surface states, doping concentration atoms ($N_D$), $R_s$ of structure, the thickness of the interfacial insulator layer and BH inhomogeneities [6, 24, 25, 27], [5, 9, 23, 31]. On the other hand, as shown in Fig. 3(b), the value of $G/\omega$ increases with voltage almost as linear for each illumination levels after 0.7V. This feature is most precisely shown at low and high illuminations and can be attributed to a conductive behavior. On the other words, when the value of C becomes decrease, $G/\omega$ value increases with increasing voltage in the accumulation region. It is clear that the minimum value of C corresponds to the maximum value of $G/\omega$ at strong accumulation region (6 V).

It is well known that in the high frequencies (f ≥ 500 kHz), the charges at surface states cannot follow the ac signal and consequently do not contribute appreciable to the PtSi/n-Si SBD capacitance. Because, the carrier life time $\tau$ is much larger than 1/(c=2πf). Therefore, in order to the frequency or polarization effect, C-V and $G/\omega$-V measurements were carried out at 500 kHz. In this case, both the possible polarization effects such surface and dipole polarizations and charges localized at surface states/interface can be eliminated low. In MS type SBDs with and without interfacial layer, the depletion layer capacitance can be expressed as [24, 27]:

$$C^{-2} = \frac{2(V_o + V)}{q\varepsilon_s A^2 N_D}$$

(4)

where $V_o$ is the built potential at zero bias and is determined from the extrapolation of the linear $C^{-2}$-V plot to the V axis, $\varepsilon_s$ is the dielectric constant of the semiconductor (=11.8$\varepsilon_o$ for Si), $N_D$ is the donor concentration atoms in Si and A is the rectifier contact area. As is shown in Fig.4 the plots of $C^{-2}$-V considered two linear parts which are corresponding to the (0.2-0.4) V and (0.6-0.8) V, respectively. With the help of Eq. (4), the values of $N_D$ can be determined from the slope of the $C^{-2}$-V plot according for two parts for each illumination level. The $C^{-2}$-V plots as a function of voltage in the region (0.2-0.4) V are linear that indicate the formation of Schottky diodes. The ionized doping concentrations of n-Si in this region were found as 9.00x10^{18} cm^{-3} (in dark and 25-100 mW/cm²) and 3.13x10^{18} cm^{-3} (under 10 mW/cm²) at room temperature and 500 kHz.

The second linear part of the C$^{-2}$-V plots indicated a different distribution of donor concentration. As can be seen in Fig.5, in the bias range of 0.6-0.8 V, doping concentrations were found as 6.20x10^{19} cm^{-3} (in dark), 2.60x10^{19} cm^{-3} (under 10 mW/cm²) and 3.76x10^{19} cm^{-3} (under 25-100 mW/cm²). These values differ from primary doping level of n-Si(111) substrate (~10^{15} cm^{-3}).

In addition, with the help of Eq.(4), the values of $V_o$ were determined from the intercept of the C$^{-2}$-V plots. Thus, the value of the BH was calculated by the following equation using the C-V measurements for each illumination level.

$$\Phi_B(C-V) = q(V_o + V_o)$$

(5)
Here: $V_n$ is the potential difference between the Fermi energy level $E_F$ and the bottom of the conduction band ($E_c$) in the neutral region of n-Si. The values of $V_n$ can be obtained as \[24, 25, 27\], \[28\]

\[ V_n = \frac{kT}{q} \ln \left( \frac{N_c}{N_D} \right) \]  

(6)

with

\[ N_c = 4.82 \times 10^{15} T^{3/2} \left( \frac{m_e^*}{m_0} \right)^{3/2} \]  

(7)

where $N_c$ is the effective density of states in nondegenerated Si conductance band ($N_c = 2.85 \times 10^{19}$ cm$^{-3}$ for Si at room temperature [24, 25, 27]), $m_e^*/m_0 = 1.09$ is the effective mass of the density of states of silicon. As can be seen in Table 1, for the range of bias voltage (0.2-0.4)V the values of $V_n$ (~0.027 eV) are practically independent of illumination. Only difference comes from the illumination level of 10 mW/cm$^2$ such that the value of $V_n$ is 0.055 eV. For the second part of C$^2$V plots (0.6-0.8 V) the value of $V_n$ changes from -0.020 to -0.006 eV for dark and illumination conductions from 25-100 mW/cm$^2$ and -0.001 for 10 mW/cm$^2$. It show, that some regions of the semiconductor are degenerated, the conduction band crosses the Fermi level. The bottom of the conduction band is located below or above the Fermi level for PtSi/n-Si (111) diodes.

The value of $\Phi_B$ (C-V) of PtSi/n-Si(111) structure was obtained from C$^2$V plots in dark and illumination levels of 10, 25, 40, 63, 80 and 100 mW/cm$^2$ as (0.54-0.56) eV and (0.87-1.082) eV for first and second parts, respectively. We believe, that the big value of barrier height caused by the existence of an inversion layer with high charge density.

Full set of calculated values of $\Phi_B$ are given in Table 1 and Fig.6. The depletion layer width $W_D$ was calculated from C-V characteristic for each illumination intensity at 500 kHz using the equation for the width of the space charge region:

\[ W_D = \left[ \frac{2e_o V_o}{qN_D} \right]^{1/2} \]  

(8)

As shown in Table 1, the depletion layer width ($W_D$) consists of two parts as $W_{D1}$ and $W_{D2}$ and changes with increasing illumination intensity [7]. The investigation of C$^2$-V plots revealed the presence of two barriers for all illumination levels for PtSi/n-Si(111) SBD. Obtained result are in good agreement with the results of previous papers [8, 14, 29, 30]. The value of potential barrier height of PtSi/n-Si(111) SBD derived from the I-V measurements is the average value of barrier height extracted from the reverse bias C-V curves, practically. The reason for the discrepancy between the barrier height values determined from C-V and I-V characteristics can be explained as following; current in the I-V measurement is dominated by the current, which flows through the region of lower patches of barrier height. This discrepancy could also be explained by the existence of an interfacial layer, trap states in the substrate, the effect of the image force and the barrier inhomogeneities at M/S interface. On the other hand, when PtSi/n-Si(111)
SBD is illuminated, the quantity of majority charges changes weakly due to double potential barrier and the contribution of tunneling [4].

According to a method presented by Nicollian and Brews [23], the real \( R_s \) of the MS and MIS structures can be calculated from the measured capacitance \( C_{ma} \) and conductance \( G_{ma} \) at the strong accumulation region [6, 9, 24, 25, 27]:

\[
R_s = G_{ma} \left( G_{ma}^2 + (\omega C_{ma}^2)^2 \right)^{-1}
\]

In this study, using Eq. (9), \( R_s \) of PtSi/n-Si structures were calculated as a function of bias at various illumination levels as shown in Fig. 7.

As seen in Fig. 7, the \( R_s \) values of the PtSi/n-Si(111) SBD reveals a peak between about 0-1.0 V such that the peak behavior is practically independent of illumination level and disappears at positive voltages (>0.7 V). The value of \( R_s \) was calculated from the any measured capacitance \( C_m \) and conductance \( G_m \), which is connected with contribution of surface states.

It is known that the formation of silicide results in displacement of M/S interface deep into the semiconductor. As a result, the pressure during the epitaxial growth process leads to the displacement of atoms from the equilibrium positions [13]. Werner and Guttler have concluded from the analysis of Schottky contacts that there is a direct influence of the interface-crystallography on both the BH and its temperature dependent [30]. In this respect, the formation and characterization of contact on Si(100) and Si(111) has been subject of a vast number of fundamental studies due to its importance as a semiconductor device in electronics [30, 32, 33]. On the other hand, it is known that crystal lattice of Si(111) contains hexagonal emptiness, areas which are about 14.6 \( \times \) \( 10^{-2} \) nm\(^2\) [29]. An important role in the formation of a film on the surface of the semiconductor plays the ratio of parameters of the contacting materials. As is revealed from the analysis of literature, films epitaxially grow, have an ordered structure similar to the single crystal and repeat structure of the substrate if the difference (mismatch) in lattice parameters does not exceed 4%. If the difference is greater than 4% at the initial stage of growth of the epitaxial film, in this case films are formed as three-dimensional islands. At the initial stage of growth these islands are small, but a high density distribution on the substrate surface [14].

The mismatch of the lattice parameters PtSi and Si is 12%, which is large enough to create a uniform contact. In addition, it is known, that in a process of epitaxial growth atoms displaced from their equilibrium positions. This results in the lattice deformation of contacting materials and is a change in the band structure of materials [13, 23]. Heavily doped silicon spots lead to a change in the spatial position of the quasi-Fermi [6, 25]. Due to the influence of the large value of the coefficient of the mismatch of lattice parameters of PtSi and silicon (Si), the emptiness that are present in the semiconductor, are filled with atoms of another substance [13].

It should be noted that the radius of Pt atom is 1.39A, radius of the Si atom is 1.17A, whereas the radius of the emptiness, assuming that it is a circular, is approximately 2.15 A [29]. These emptiness can be filled with atoms of platinum. Thus, there are formed spots with a high degree of doping, which contribute to local narrowing of the space charge region of PtSi/n-Si(111) diodes.
The behaviour of the barrier heights being larger than the band gap energy has been explained by some researchers, as being due to the existence of an inversion layer with high charge density [18].

Based on this result, it has been concluded that the presence of these emptiness in crystal structure Si(111) increases the probability of inhomogeneous formation of spots and the presence of two barriers at PtSi/n-Si(111) metal-semiconductor contact [7].

4. Conclusions

Both the forward and reverse bias I-V characteristics of PtSi/n-Si (111) (MS) type SBDs have been investigated both in dark and under various illumination intensities at room temperature. While the forward bias lnI-V characteristics of the diode are almost independent on illumination level, but the reverse bias lnI-V characteristics were found a strong function of due to high electric field in the junction. The values of ideality factor $n$ and saturation current $I_0$ were found as 1.22 and $2 \times 10^{10}$ A in dark, 1.57 and $1 \times 10^9$ A under 100 mW/cm$^2$, respectively. The values of $\Phi_{Bo}$ were calculated as 0.71 eV and 0.67 eV for in dark and under 100 mW/cm$^2$, respectively. As shown, the main value of the electrical parameters of the structure such as $\Phi_{Bo}$, $n$, $I_0$ are considerably dependent of illumination due to the basic current transport mechanism across the MS interface is the illuminated assisted tunneling.

The forward and reverse bias C-V and G/ω-V characteristics of PtSi/n-Si (MS) type SBDs have been investigated both in dark and under various illumination intensities at room temperature. The values of $R_s$ were calculated using methods of Nicollian and Brews. Sharp jump of C-V and G/ω was observed for each illumination level ($V \geq 0.7V$), whose intensity gets slightly stronger as the illumination is increased. The C$^2$-V plot has two linear regions with different slopes in the bias regions of (0.2-0.4) V and (0.6-0.8) V, respectively. The values of $N_D$, $\Phi_B$, and $W_D$ were determined from the slope of the C$^2$-V plots for these regions under various illumination levels, respectively. The values of $N_D$, $V_0$, $\Phi_B$(C-V) and $W_D$ were obtained from the intercept and slope of C$^2$-V plot in dark and under illumination conductions. As a result, it has revealed that, due to formation of silicide/n-Si interface in semiconductor, displacement of atoms from the equilibrium positions and hexagonal emptiness of crystal lattice of Si(111) doping degree of real depletion layer($\sim 10^{10}$ cm$^{-3}$) differ from primary doping level of n-Si(111) substrate ($\sim 10^{15}$ cm$^{-3}$). The width of depletion layer chances from $1.4 \times 10^6$ to $8.5 \times 10^{-7}$ cm. In addition, have been revealed two barrier, the height of which chanced from 0.54 to 1.06eV. The biq value of barrier height caused by the existence of an inversion layer with high charge density. The changing of $V_n$ from $2.7 \times 10^{-2}$ to $-2.0 \times 10^{-2}$ eV show, that due to some regions of the semiconductor are degenerated, the conduction band crosses the Fermi level and bottom of the conduction band is located below or above the Fermi level for PtSi/n-Si (111) diodes.
Obtained result indicates that, the in-homogeneities distribution of doping degree strongly influences on the electrical parameters of PtSi/n-Si(111) SBD under illumination due to PtSi formation process.

Fig. 1. (a) The structure of the fabricated chip and (b) cross section of PtSi/n-Si (111) with diffusion barrier.

Fig. 2. The lnI-V characteristics of PtSi/n-Si structure in dark and under 100 mW/cm² illumination and scattering room illumination at room temperature.
Fig. 3. (a) The C-V (a) and (b) G/ω-V (b) characteristics of PtSi/n-Si(111) structure at 500 kHz for various illumination levels.
Fig. 4. $C-V$ characteristics of PtSi/n-Si(111) SBD with diffusion barrier in dark and under various illumination intensities at 500 kHz and room temperature.

Fig. 5. The distribution of $N_D$ of n-Si in dark and under various illumination levels (10, 25, 40, 63, 80 and 100 mW/cm$^2$) vs. the depletion layer width $W_D$ for PtSi/n-Si(111) structure with diffusion barrier.
Fig. 6. The distribution of $\Phi_0(C-V)$ vs depletion layer width $W_0$ of PtSi/n-Si(111) structure in dark and under various illumination levels (10, 25, 40, 63, 80 and 100 mW/cm$^2$).

Fig. 7. The variation of the $R_s$-V plots of PtSi/n-Si structure obtained at 500kHz for in dark and under various illumination levels.
Table 1. The obtained some main electrical parameters from the $C^2$-V plots of the PtSi/n-Si(111) structure in dark and under various illumination intensities.

<table>
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<th>$P$ (mW/cm$^2$)</th>
<th>$V_{01}$ (V)</th>
<th>$V_{02}$ (V)</th>
<th>$V_{n1}$ (eV)</th>
<th>$V_{n2}$ (eV)</th>
<th>$\Phi_{B1}$ (eV)</th>
<th>$\Phi_{B2}$ (eV)</th>
<th>$W_{D1}$ (cm)</th>
<th>$W_{D2}$ (cm)</th>
<th>$N_{D1}$ (cm$^{-3}$)</th>
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<tr>
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References


