Growth and interface properties of Au Schottky contact on ZnO grown by molecular beam epitaxy

M Asghar1,3, K Mahmood1, Faisal Malik1 and M A Hasan2
1Department of Physics, The Islamia University of Bahawalpur, 63100, Pakistan
2Department of Electrical and Computer Engineering, UNC-Charlotte, NC 28223, USA
E-mail: mhashmi@iub.edu.pk

Abstract. In this paper, we have discussed the growth of ZnO by molecular beam epitaxy (MBE) and interface properties of Au Schottky contacts on grown sample. After the verification of structure and surface properties by X-Ray Diffraction (XRD) and Scanning Electron Microscope (SEM), respectively, Au metal contact was fabricated by e-beam evaporation to study contact properties. The high value of ideality factor (2.15) and barrier height (0.61 eV) at room temperature obtained by current-voltage (I-V) characteristics suggested the presence of interface states between metal and semiconductor. To confirm this observation we carried out frequency dependent capacitance-voltage (C-V) and conductance-voltage (G-V) demonstrated that the capacitance of diode decreased with increasing frequency. The reason of this behavior is related with density of interface states, series resistance and image force lowering. The C-V plot drawn to calculate the carrier concentration and barrier height with values 1.4×1016 cm⁻³ and 0.92 eV respectively. Again, high value of barrier height obtained from C-V as compared to the value obtained from I-V measurements revealed the presence of interface states. The density of these interface states (Dit) was calculated by well known Hill-Coleman method. The calculated value of Dit at 1 MHz frequency was 2×10¹² eV⁻¹ cm⁻². The plot between interface states and frequency was also drawn which demonstrated that density of interface states had inverse proportion with measuring frequency.

1. Introduction
ZnO is a material of current research due to its superior optoelectronic and nano-electronic properties which makes it ideal candidate for short wavelength ultraviolet light emitting diodes and photo-detectors [1-2]. To realize these devices for particle applications, high quality Ohmic and Schottky metal contacts are indispensible. But good Schottky contacts are difficult to fabricate due to the presence of interface states between film and substrate which can lead to a large deviation from the ideal behavior. Furthermore different metal such as Al, Au, Ag, Pt and

3 To whom any correspondence should be addressed.
Pd had been used by researchers to achieve reliable Schottky contacts. These Schottky contacts have barrier heights in the range of 0.6 eV to 0.8 eV indicating the non-negligible impact of interface defect states [3-5]. Moreover these interface states strongly depend upon the defect density of grown film and consequently on growth technique used [6]. Therefore the characterization of these interfaces states between semiconductor and metal contact is highly desirable.

In this paper, we have investigated the effect of interface states on Au Schottky diode contact fabricated on MBE grown ZnO. I-V measurements yielded ideality factor and barrier height to be 2.15 and 0.6 eV, respectively. C-V and G-V measurements performed for a wide frequency range (10 kHz – 2 MHz) at room temperature. The lower value of capacitance at higher frequencies and higher value of barrier height obtained from data C-V as compared to the one from I-V, confirmed the presence of interface states. X-ray diffraction and SEM measurements additionally performed to access the structural and surface properties of grown sample.

2. Experimental
ZnO thin film is grown on p-type silicon wafer by MBE. The detail of growth can be seen elsewhere [7]. After growth Au metal was evaporated by e-beam evaporation to form metal contacts of diameter 1 mm.

3. Results and discussion
Figure 1 is typical XRD pattern of grown ZnO film. It shows three peaks at 2θ angles 34°, 36° and 72° corresponding to ZnO (002), (101) and (004) planes, respectively. The full width half maximum of ZnO (002) peak is 0.3°. This small value of FWHM demonstrates the good quality of film.

![Figure 1](image_url)  
**Figure 1.** XRD pattern of as-grown ZnO thin film on silicon substrate indicating that preferred growth orientation is along C-axis.
The thermionic emission theory for a bias voltage, $V$, is valid for the analysis of electrical characteristics of the Schottky barrier structures of Au/ ZnO/p-Si, and hence junction current can be expressed by [8]

$$I = I_s \left[ \exp\left(\frac{qV}{nkT}\right) - 1 \right]$$  \hspace{1cm} (1)

where $n$ is the ideality factor and $I_s$ is the reverse saturation current given by,

$$I_s = A^* A T^2 \exp\left[\frac{-q\Phi_{ap}}{kT}\right]$$  \hspace{1cm} (2)

where $A$ is diode area, $A^*$ is Richardson’s constant, $q$ is charge, $\Phi_{ap}$ is apparent barrier height, $k$ is Boltzmann’s constant and $T$ is temperature.

![Current-Voltage characteristics of Ni/ZnO/Si Schottky diode at room temperature.](image)

**Figure 2.** Current-Voltage characteristics of Ni/ZnO/Si Schottky diode at room temperature.

The ideality factor ($n$) of Schottky barrier is an important parameter that explains the perfection of metal-semiconductor junction. It is determined from the slope of semilog $I$-$V$ (not shown here) characteristics in the exponential region by the relation;

$$n = \frac{q}{kT \times slope}$$  \hspace{1cm} (3)

where $q$ is the charge (C), $k$ is Boltzmann’s constant (J/K), $T$ is Temperature (K) [9]. The measured value of ideality factor at room temperature for Au/ZnO Schottky diode is 2.15. The
high values of $n$ can be attributed to effects of the bias voltage drop across the interfacial layer and series resistance.

The barrier height is an electrostatic barrier to the charge transfer across the metal/semiconductor interface. The barrier height $\phi_b$ can be written as

$$\phi_b = \frac{kt}{q \ln \left( \frac{A' T^2}{I_s} \right)} \quad (4)$$

where $k$ is Boltzmann’s constant ($J/K$), $T$ is temperature ($K$), $q$ is charge of electron ($C$), $A$ is Schottky contact area ($cm^2$), $A'$ is Richardson constant ($J/cm^2 K$) and $I_s$ is reverse saturation current ($A$). The barrier height can be determined by the intercept of the linear part of the forward bias voltage at exponential (region not shown here). The measured value of barrier height for Au/ZnO/Si Schottky contact is 0.6 eV and it is well agreed with the reported value.

![Figure 3. Plot of C-V of Ni/ZnO/Si Schottky contact at different frequencies.](image)

Figure 3 is typical C-V characteristics of Au/ZnO/Si Schottky diode between voltage range of -4 V to +5 V at room temperature and at different frequencies ranging from 10 kHz to 2 MHz. The graph shows that the value of capacitance is decreasing with increasing frequency and plot exhibits a peak in positive voltage. This peak is gradually disappeared as frequency increased from 10 kHz to 2 MHz. The possible reasons of this peak may the presence of deep states in the band gap, series resistance and interface density states [10].
C - V characteristics can be analyzed by plotting \(1/C^2\) vs V and deducing \(N_d\) from the slope and \(V_{bi}\) from the intercept of reversed biased capacitance-voltage (C-V) characteristics using following equation.

\[
N_d = \frac{-2}{q \varepsilon_0 \varepsilon_r \left(\frac{A}{C}\right)^2} \left(\frac{d(A/C)^2}{dv}\right)
\]

Where \(q\) (\(1.6 \times 10^{-19}\) C) is the charge on an electron, \(\varepsilon_0\) (\(8.85 \times 10^{-14}\)) is the permittivity of the free space, \(\varepsilon_r\) (=9.66) is the relative permittivity of the medium, \(A\) is the area of the Schottky contact (0.034cm\(^2\)) and \(C\) is the capacitance in pF.

The measured value of doping concentration at 2 MHz frequency is \(1.4 \times 10^{16}\) cm\(^{-3}\). The barrier height value can also be deduced from this graph. The barrier height obtained from reversed biased \((A/C)^2\) graph is 0.91 at 1 MHz frequency. The measured value of barrier height from C-V characteristics is high as compared to barrier height extracted from I-V data. This difference is due to the presence of interface states at interface and other possible reasons may be barrier height inhomogenity and image force lowering.

Figure 4. \(C^2\) - V characteristics of Au / ZnO / Si Schottky diode at different frequencies.
Figure 5. Frequency dependent plot of capacitance of Au / ZnO / Si Schottky diode at different biases.

Generally the capacitance measured for the rectifying contact is dependent on the reverse bias voltage and frequency. Its voltage and frequency dependence is due to the particular features of a Schottky barrier, impurity level, high series resistance, interface states and interface layer between Au and ZnO. This dependence of capacitance on frequency is shown in figure 5. The higher values of capacitance at low frequency are due to the excess capacitance resulting from the interface states in equilibrium with the n-type ZnO that can follow the ac signal. At low frequency the measured capacitance is dominated by the depletion capacitance of the rectifying contact, which is bias-dependent and frequency-independent. As the frequency is increased, the total diode capacitance is affected not only by the depletion capacitance, but also the bulk resistance which is frequency-dependent and associated with electron emission from slowly responding deep impurity levels. Furthermore at high frequencies the interface states cannot contribute to capacitance because the charge at the interface states cannot follow the a.c signal, therefore the capacitance at high frequencies is low as compared to low frequencies [11].
Figure 6. Conductance-Voltage (G-V) characteristics of Au / ZnO / Si Schottky diode at different frequencies.

Figure 6 shows the G - V characteristics of Au/ZnO/Si Schottky contact at different frequencies and room temperature. The conductance of device is decreased as frequency increased. This behavior of conductance is attributed to particular distribution of interface states. From this plot it is also evident that positive voltage the conductance remained almost for all frequencies. Therefore it is concluded that at negative voltages the interface states are responsible of this conductance dispersion.

Figure 7. Frequency verses Dit plot of Au / ZnO / Si Schottky diode.
The density of interface states can be determined by Hill-Coleman method [12]. According to this method \(D_{it}\) can be calculated by the following formula

\[
D_{it} = 2G_{c,\text{max}}/w \cdot qA \left[\left(G_{c,\text{max}}/wC_{\text{ox}}\right)^2 + \left(1 - C_{c}/C_{\text{ox}}\right)^2\right]
\]  (6)

Where \(A\) is the diode area, \(q\) is electronic charge, \(w\) is angular frequency, \(C_{\text{ox}}\) is the capacitance of oxide layer in accumulation region of C-V curves, \(G_{c,\text{max}}\) maximum conductance of G-V curve and \(C_{c}\) is the capacitance of diode corresponding to \(G_{c,\text{max}}\).

Figure 7 shows the density of interface states verses frequency. The calculated value of \(D_{it}\) values decrease with increasing frequency. Similar results have been published in references.

4. Conclusion
The properties of interface have been demonstrated with the help of I-V and C-V measurements of Au/ZnO/Si Schottky diode. The ideality factor and barrier height of diode was calculated by I-V measurements at room temperature with values 2.15 and 0.61 eV respectively. Frequency dependent C-V and G-V measurements performed to access the density of interface. Non ideal behavior of measured parameters suggested the presence of interface states. These interface states were calculated by famous Hill-Coleman method. The measured density of interface states is enough to strongly degrade the performance of device.

Acknowledgements
Authors are thankful to Higher Education Commission Pakistan for financial support under project No. 624/2007. The authors are also thankful to UNC-Charlotte, USA for technical support.

References
[1] Zou C W, Wang H J, Yi M L, Li M, Liu C S, Guo L P, Fu D J and Kang T W 2010 Appl. Surf. Sci. 256 2453
[2] Asghar M, Mahmood K and Hasan M A 2012 Key Eng. Mat. 511-512 132
[3] Karadeniz S, Tugluoglu N, Serin T and Serin N 2005 Appl. Surf. Sci. 246 30
[4] Karadeniz S, Tugluoglu N, Serin T and Serin N 2004 Appl. Surf. Sci. 233 5
[5] Cova P and Sing A 1990 Solid-State Electon. 33 11
[6] Songul D, Emre G, Syedi D and Sebahattn T 2009 Current Appl. Phys. 9 1181
[7] Asghar M, Mahmood K and Hasan M A 2012 Key Eng. Mat. 511-512 227
[8] Card H and Rodrick EH 1971 J. Phys.; D 4 1589
[9] Wenksten H V, Kaidashev E M, Lorentz M, Hochmuth H, Biehne G, Lenzer J, Gottscalch V, Pickenhain R and Grundmann M 2004 Appl. Phys.Lett. 84 79
[10] Nicollian E H and GoetzbergerA 1967 Bell Syst. Tech. J. 46 1055
[11] Sing A 1985 Solid-State Electron. 28 233
[12] Hill W A and Coleman C C 1980 Solid-State Electron. 23 987