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Metal Contacts on a-GaN

T. U. Kampen, W. Mönch
Laboratorium fuer Festkoerperphysik, Gerhard-Mercator-Universitaet Duisburg

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Abstract

The Schottky barrier heights of silver and lead contacts on *n*-type GaN (0001) epilayers were determined from current-voltage characteristics. The zero-bias barrier heights and the ideality factors were found to be linearly correlated. Similar observations were previously reported for metal contacts on Si (111) and GaAs (110) surfaces. The barrier heights of ideal Schottky contacts are characterized by image force lowering of the barrier only. This gives an ideality factor of 1.01. From our data we obtain barrier heights of 0.82 eV and 0.73eV for ideal Ag and Pb contacts on GaN, respectively. The metal-induced gap states (MIGS) model predicts the barrier heights of ideal Schottky contacts on a given semiconductor to be linearly correlated with the electronegativities of the metals. The two important parameters of this MIGS-and-electronegativity model are the charge neutrality level (CNL) of the MIGS and a slope parameter. The CNL may be calculated from the dielectric band gap and using the empirical tight-binding method. The slope parameters are given by the optical dielectric constant of the respective semiconductor. The predictions of the MIGS model for metal/GaN contacts are confirmed by the results presented here and by barrier heights previously reported by others for Au, Ti, Pt, and Pd contacts on GaN.

1. Introduction

Most metal-semiconductor contacts are rectifying. The electronic transport across such Schottky contacts is characterized by their barrier heights. The barrier height is the energy distance between the Fermi level W_F and the respective majority carrier band edge at the interface (respectively, the valence-band maximum W_{vi} for *p*- and the conduction-band minimum W_{ci} for *n*-type semiconductors). The famous Schottky-Mott rule [1] [2] predicts the barrier height to be equal to the difference between the electron affinity of the semiconductor and the work function of the metal. Schweikert (see [3]) was the first to test this rule. He found the barrier heights of metal-Se contacts to vary proportional to the work functions of the metals used but with a slope much smaller than unity. This strong deviation from what is predicted by the Schottky-Mott rule was explained by interface states [4]. At metal-semiconductor interfaces, the wavefunctions of the metal electrons decay exponentially into the semiconductor in the energy range where the metal conduction band overlaps the semiconductor band gap. These wavefunction tails form the continuum of the metal-induced gap states (MIGS) [5] which are the intrinsic interface states in such contacts.

The character of the metal-induced gap states varies across the bandgap from mostly donor-like to predominantly acceptor-like closer to the valence and the conduction band, respectively. When the respective branch point is above, coincides with, or below the Fermi level, then the corresponding net charge-density in the metal-induced gap states is positive, zero, or negative.Therefore, these branch points are also called the charge neutrality levels (CNL) of the MIG states. The energy position of the Fermi level at a metal-semiconductor interface, and by this its barrier height, depends on the occupation of the MIGS.

Interfaces are electrically neutral. Therefore, the charge densities on both sides of an interface are of equal magnitude but opposite sign. Pauling [6] described the ionicity of diatomic molecules by the difference of the atomic electronegativities. A generalization of this concept models the charge transfer across metal-semiconductor interfaces by the difference $X_m - X_S$ of the electronegativities of the metal and thesemiconductor in contact.

The MIGS-and-electronegativity model predicts barrier heights to vary as [7]

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$$\phi_{Bn} = \phi_{cnl} + S_x (X_m - X_s) \quad (1)$$

on semiconductors doped *n*-type. The zero-charge transfer barrier height $\phi_{cnl} = W_{ci} - W_{cnl}$ results when the electronegativity difference $X_m - X_s$ is zero. As a consequence of this, the Fermi level coincides with the charge neutrality level of the MIGS. The MIGS-and-electronegativity model predicts the barrier heights of ideal metal-semiconductor contacts to be determined by two parameters: the energy position $W_{cnl} - W_v(\Gamma)$ of the charge neutrality level of the MIGS with regard to the valence-band maximum and the slope parameter $S_x = \partial\phi_{Bn} / \partial X_m$.

The MIG states represent the *primary* mechanism which determines the barrier heights in ideal, i.e., intimate, abrupt, defect-free, and laterally homogenous metal-semiconductor contacts. Deviations from what is predicted by the MIGS are then caused by *secondary* mechanisms, e.g. interface dipoles induced by specific interface structures or layers of foreign atoms and interface defects [8].

Research on both ohmic and Schottky contacts are of current interest for GaN. Khan *et al.* [9] measured 0.91 eV Schottky barrier height for Au/GaN contacts. The barrier heights of Ti and Au contacts on GaN were determined by Binari *et al* to be 0.59 eV and 1.19 eV, respectively [10]. For Pt and Pd contacts, barrier heights of 1.04 eV and 0.94 eV, respectively, were reported [11].

In the present study, Pb and Ag were evaporated on *n*-type α-GaN epilayers grown on sapphire. These contacts are rectifying.Their zero-bias barrier heights ϕ_{Bn}^0 were evaluated from the current-voltage (*I/V*) characteristics. Our experimental data and those previously published by others are analyzed by applying the MIGS-and-electronegativity model.

2. Experimental

The substrates used were cut from *n*-type α-GaN epilayers on sapphire (Cree Research Inc.). The doping level of these layers is below 5×10^{16} cm^{-3}. The following cleaning procedure was applied. The samples were first dipped for 1 min into hydrofluoric acid which was then diluted by a buffered HF-solution ($HF:NH_4F:NH_4OH$) having pH = 9, then rinsed in de-ionized water, blown dry with N_2 gas, and transferred into the UHV system. There they were heated to a temperature of about 800° C and simultaneously exposed to a Ga flux with a rate of 1×10^{16} cm^{-2} s^{-1}. The Ga flux was shut off after 10 min of exposure and the samples were further heated for 30 min. The surface cleanliness was checked by photoemission excited with Mg(Kα) radiation. The spectra recorded showed no trace of residual surface impurities. All surfaces showed sharp 1×1 LEED patterns.

After surface preparation, Pb or Ag was evaporated onto the clean GaN surfaces from Knudsen cells. In front of the samples a mask was placed which had circular openings with nominal diameters of approximately 1 mm. The exact diameter of the diodes was evaluated by using a microscope. The metal evaporation rate was monitored by a quartz-crystal thickness monitor and adjusted to 0.05 nm/s. Usually, a total of 150 nm of metal was deposited. The *I/V* measurements were performed outside the UHV system at room temperature in the dark. Ohmic contacts were achieved by rubbing Ga into the GaN with an Al-pencil.

3. Results

The Ag and Pb/*n*-α-GaN contacts were always rectifying. Figure 1 shows the forward *I/V* characteristics of one diode each at T=296 K. For thermionic emission over the barrier the current density of Schottky contacts as a function of applied voltage V_a is given by [12],

$$j = A^{**}T^2 \exp(-\phi_{Bn}^0 / k_B T) \exp(e_0 V_a / n k_B T)[1 - \exp(-e_0 V_a / k_B T)] \quad (2)$$

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where n is the ideality factor, A^{**} is the effective Richardson constant, and k_B and e_0 are Boltzmann´s constant and the elementary charge, respectively. The effective mass of the conduction electrons in GaN, $m^* = 0.22\ m_0$ [13], gives an effective Richardson constant $A^{**} = 26.4 \times 10^4$ A/cm^{2}K. This value is used here. For applied voltages larger than $3k_BT/e_0 \approx 0.08$ V the data displayed in Figure 1 exhibit the semilogarithmic behavior expected from equation 2. The deviation from the straight line for applied voltages larger than 0.15 V is due to the sample series resistance, the back contact, and the external electrical connections. Least-squares fits of equation 2 to the linear portions of the *I/V* curves shown in Figure 1 give barrier heights of 0.7 eV and 0.72 eV and ideality factors of 1.57 and 1.28 for the Ag and the Pb contacts, respectively.

Barrier heights and ideality factors vary from diode to diode. However, a linear correlation between both quantities was observed for Ag/S/*n*-GaAs(001) [14], Ag/*n*-Si(111)-"7×7", Ag/*n*-Si(111)-1×1 [15], Ag/*n*-Si(111):H-1×1 [16], Pb/H:*p*-Si(111) and Pb/*n*-Si(111) Schottky diodes [8]. Therefore, the barrier heights of all our Ag- and Pb/*n*-αGaN contacts are plotted in Figure 2 versus their ideality factors. The straight lines are least-squares fits to the data.

4. Discussion

Tung [17] studied the potential distribution and the current transport in Schottky contacts with non-uniform barrier heights along the interface. He calculated effective barrier heights and ideality factors of such patchy contacts as a function of the shape and size of the inhomogeneities and the deviations of their barrier heights from the value of the homogenous interface. A combination of two relations derived by Tung indeed gives a linear correlation between effective barrier heights and ideality factors of nonuniform contacts. Interface defects, for example,may induce a non-uniform distribution of barrier heights and increase the ideality factor.

The barrier height of homogeneous metal-semiconductor contacts are lowered and become voltage-dependent due to the image-force or Schottky effect. For the GaN samples used the respective ideality factor results as n_{if} =1.01 [15] [16].The extrapolation of the least-squares fits in Figure 2 to this ideality factor gives zero-bias barrier heights of 0.82 eV and 0.73 eV for uniform Ag and Pb contacts, respectively. The two important parameters of the MIGS-and-electronegativity model are the CNL and the slope parameter. The slope parameters are given by the optical dielectric constant ε_∞ of the respective semiconductor [18]

$$A_x / S_x - 1 = 0.1(\varepsilon_\infty - 1)^2 \tag{3}$$

The parameter A_x = 0.86 accounts for the use of Miedema's electronegativity scale. The MIG states derive from the virtual gap states of the complex semiconductor band structure. Their branch points are given by [19] [20]

$$W_{bp} - W_v(\Gamma) = 0.446 W_{dg} - [W_v(\Gamma) - W_v(\vec{k}_{mv})]_{\mathrm{EIB}} \tag{4}$$

where W_{dg} is the dielectric band gap [21] and $[W_v(\Gamma) - W_v(\vec{k}_{mv})]_{\mathrm{ETB}}$ is the position of the valence band at the mean-value or Baldereschi point $\vec{k}_{mv}$ in the Brillouin zone [22] with regard to the valence band maximum. This energy difference is calculated using the empirical tight-binding method. Equation 4 was derived for zincblende-structure semiconductors.

From equations (3) and (4) one obtains a slope parameter S_x = 0.29 eV/Miedema-unit. and $W_{bp} - W_v(\Gamma)$ = 2.35 eV for cubic ß-GaN. However, the barrier heights reported here and by others [9] [10] [11] were all obtained with wurtzite rather than zincblende GaN. SiC is another example for such polytypism. Barrier heights were reported for Schottky contacts on the cubic 3C- and hexagonal 6H-SiC. Mönch [23] analyzed these data and found the energy position of the CNL with regard to the valence band maximum to be the same with both SiC polytypes.Therefore, the positions of the CNLs in β- and α-GaN with regard to the valence band maximum are also assumed to be identical.

Figure 3 displays the barrier heights of uniform Ag and Pb contactson *n*-type α-GaN which were obtained by extrapolation of the experimental data to n_{if} = 1.01. The MIGS line of GaN, which results from equations (3) and (4)

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extrapolation of the experimental data to $n_{if} = 1.01$. The MIGS line of GaN, which results from equations (3) and (4), is also shown in Figure 3. The Ag and Pb/GaN data agree with the predictions from the MIGS model. Therefore, these values are characteristic not only of uniform but also of ideal α-GaN Schottky contacts. Figure 3 also displays the experimental data published by Khan *et al.* [9], Binary *et al.* [10], and Guo *et al.* [11]. These data also confirm the predictions of the MIGS-and-electronegativity model. From Figure 3 it follows that ideal metal-GaN contacts are rectifying. In this respect GaN exhibits the same behavior as almost all metal-semiconductor contacts. Genuinely ohmic contacts are only observed with metal contacts on *n*-InAs and *p*-GaSb. Therefore, ohmic contacts on GaN require specific preparational methods which e.g. produce tunnel contacts with apparently ohmic *I/V* characteristics.

Acknowledgments

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Figures

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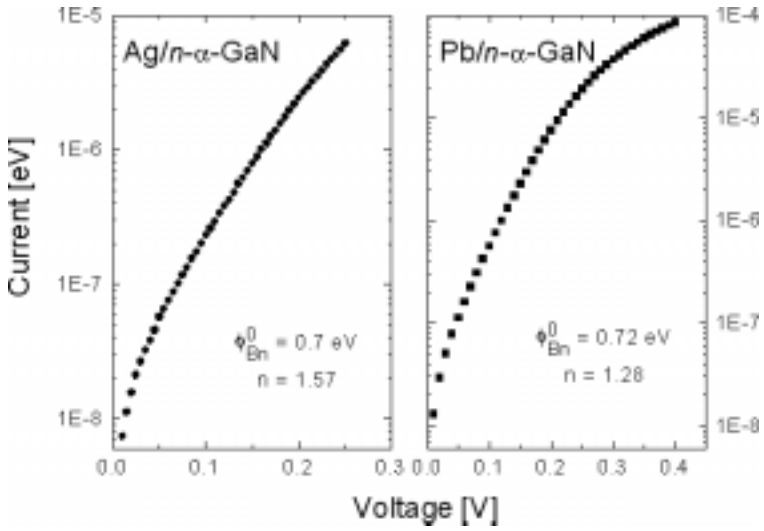

Figure 1. *I*/*V*characteristics of Ag- and Pb/*n*-α-GaN Schottky diodes at room temperature.

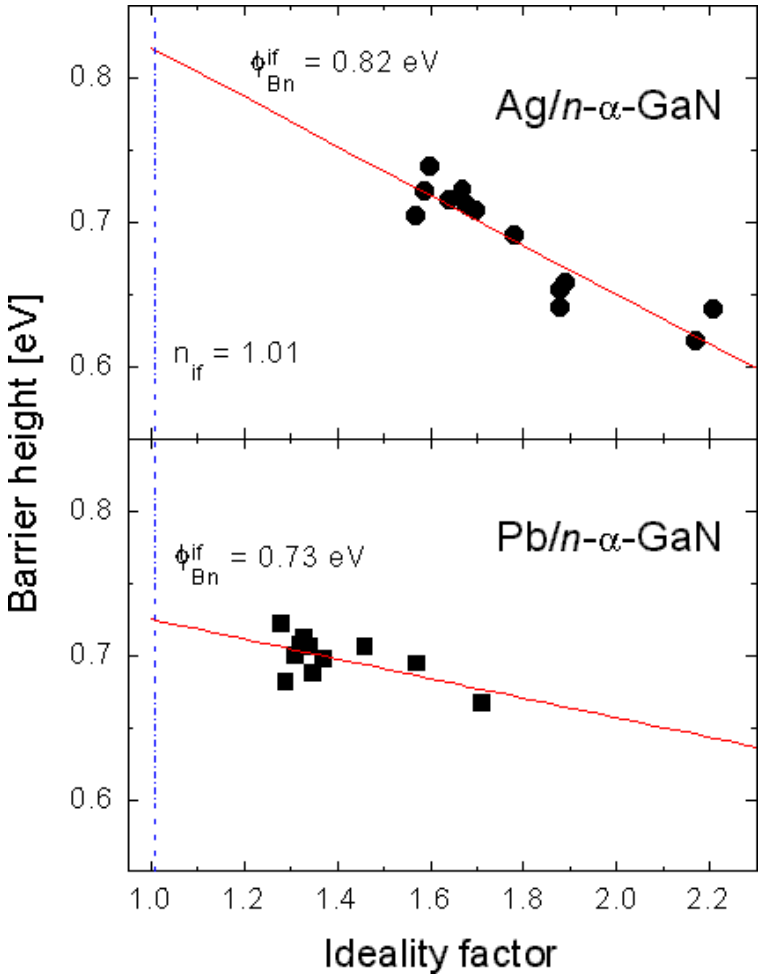

Figure 2. Zero-bias barrier heights of Ag- and Pb/*n*-α-GaN Schottky diodes as a function of the respective ideality factor.

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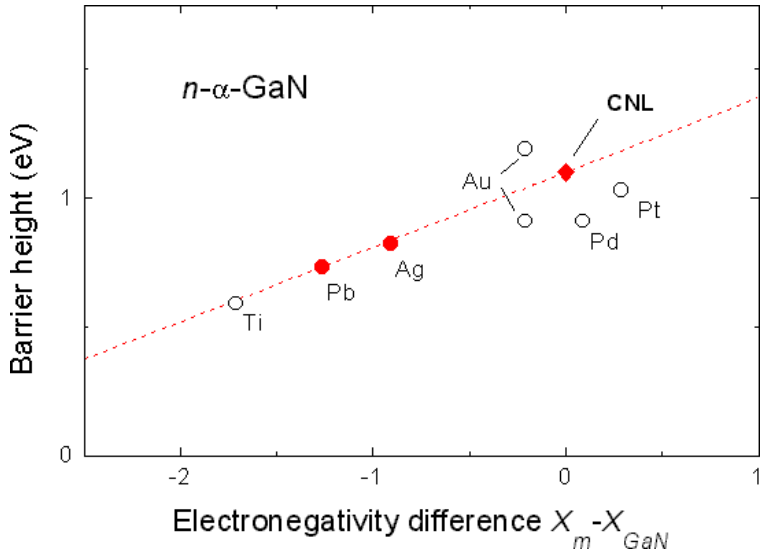

Figure 3. Barrier heights of α-GaN Schottky contacts as a function of the electronegativity difference $X_m - X_{GaN}$. (O) data from Refs. [14], [15], [16].

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