COMMENTS

Comment on “Influence of crystal polarity on the properties of Pt/GaN Schottky diodes” [Appl. Phys. Lett. 77, 2012 (2000)]

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Because of its uniaxial wurtzite structure GaN exhibits new interesting electronic properties as compared with classical, cubic III–V semiconductors. Many of these properties are due to the built-in strong polarization fields, spontaneous, and in addition, piezoelectric ones in the case of strained layers. In this context, Karrer *et al.*[1] report about differing Schottky-barrier heights of Pt/GaN contacts measured on molecular-beam epitaxy grown n-GaN layers with Ga- and N-face polarity. From capacitance–voltage and current–voltage measurements, the authors derive barrier heights $\Phi_{\mathrm{exp}}(\mathrm{Ga-face})=1.1$ eV and $\Phi_{\mathrm{exp}}(\mathrm{N-face})=0.9$ eV for GaN(0001) and GaN(000$\bar{1}$), respectively. The interpretation of the authors for this obvious difference is in terms of a different band bending on the two polar faces, inferred from a different screening behavior of the internal polarization charges at the surfaces. This different band bending is claimed to lead to different electron affinities at the two surfaces and therefore different Schottky-barrier heights.[1]

There are two fundamental errors in this interpretation:

(1) Surface band bending in a semiconductor does not affect the electron affinity of the semiconductor, apart from possible higher order effects; and
(2) the band bending under the Schottky contact is primarily determined by the metal-induced gap states (MIGS)[2,3] and not by the clean surface properties.

Different screening behavior of the polarization charges on the clean GaN surfaces, in terms of semiconductor space charge, can therefore not explain the measured difference in Schottky-barrier heights for both GaN polarities, as is assumed by Karrer *et al.*[1]

In this comment, we propose an interpretation of the experimental results[1] in terms of different polarization interface charges entering the charge balance at the Pt/GaN interface, which is based on the MIGS model by Heine,[4] Tersoff,[5] and refined by Mönch.[2]

Figure 1 shows experimentally determined Schottky-barrier heights for several metals that obey, according to Mönch,[3] the “refined” MIGS theory which takes into account bonding charge transfer at the interface expressed in terms of the electronegativity difference between metal and the GaN substrate. Using the Miedema electronegativity values 5.65 and 5.36 for Pt and GaN, respectively, the Schottky-barrier heights measured by Karrer *et al.*[1] (dots for Pt in Fig. 1) deviate from the MIGS model curve with $\Phi_{\mathrm{exp}}(\mathrm{N-face}) < \Phi_{\mathrm{exp}}(\mathrm{Ga-face}) \leqslant \Phi_{\mathrm{Bn}}$.

Except for the N-face point measured by Karrer *et al.*,[1] all other experimental points have been derived for Schottky contacts on the GaN(0001) surface (Ga-face).

Let us first discuss the Pt(N-face) Schottky barrier, which mostly deviates from the predicted value $\Phi_{\mathrm{Bn}}=1.18$ eV. The interface as a whole has to be electrically neutral and in GaN also the polarization charge close to the surface, $Q_{\mathrm{pol}}>0$ for the N-face polarity, enters the interface charge balance:

$$Q_m + Q_s = Q_m + Q_{\mathrm{gs}}^{\mathrm{mi}} + Q_{\mathrm{sc}} + Q_{\mathrm{pol}} = 0, \tag{1}$$

where Q_m and Q_s are the charges in the metal and the semiconductor, and $Q_{\mathrm{gs}}^{\mathrm{mi}}$ and Q_{sc} those in MIGS and in the space charge layer, respectively.

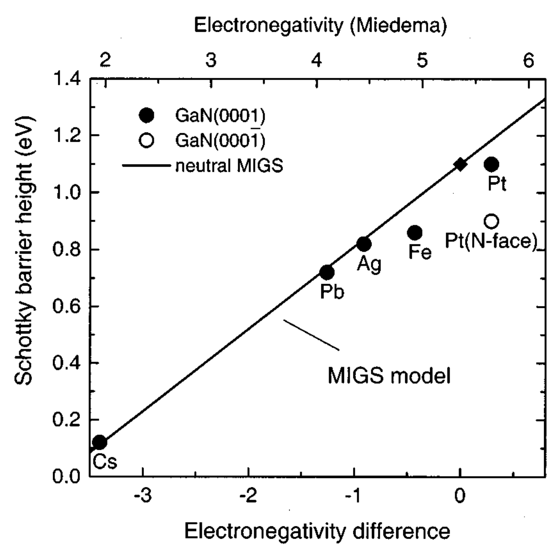

FIG. 1. Barrier heights of laterally homogeneous GaN Schottky contacts as a function of the difference of the metal and the GaN electronegativity. The MIGS line is drawn after $\Phi_{\mathrm{Bn}}=\Phi_{bp}+S_X(X_m-X_s)$ with $\Phi_{bp}=1.1$ eV and $S_X=0.29$ eV/Miedema unit, derived from a charge neutrality condition, which does not take into account the polarization charge close to the GaN surface (after Ref. 3).

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Following the calculation of Mönch [Ref. 3 and Eqs. (23) and (24)] the deviation from the MIGS model in Fig. 1 can be expressed as

$$D_{gs}^{mi}[\Phi_{Bn} - \Phi_{Bn}(\mathrm{N-face})] = Q_{pol}/e + \Delta Q_{sc}/e, \qquad (2)$$

where ΔQ_{sc} is the difference of the semiconductor space charge, due to the different Schottky-barrier heights, $\Phi_{Bn}=1.18$ eV and $\Phi_{exp}(\mathrm{N-face})=0.9$ eV. Within the simple Schottky model $Q_{sc}/e \simeq 3\times10^{12}\ \mathrm{cm}^{-2}$ and $\Delta Q_{sc}/e=4\times10^{11}\ \mathrm{cm}^{-2}$ with $\epsilon_{GaN}=9.5$ and $N_D=8\times10^{17}\ \mathrm{cm}^{-3}$ as in Ref. 1. Using theoretical data for the spontaneous polarization of GaN,[6] the absolute amount of Q_{pol}/e is obtained as $1.8\times10^{13}\ \mathrm{cm}^{-2}$, and therefore, we neglect the small difference of the space charge, as compared with Q_{pol} in Eq. (2). We thus end up with

$$\Phi_{Bn} - \Phi_{Bn}(\mathrm{N-face}) = 0.33\ \ \mathrm{eV} \qquad (3)$$

as the difference between the model Schottky-barrier height (continuous line in Fig. 1) and the calculated value, once the positive polarization charge has been added to the model. The density of MIGS around the Fermi level D_{gs}^{mi} has been calculated to be $D_{gs}^{mi}=5.43\times10^{13}\ \mathrm{cm}^{-2}\,\mathrm{eV}^{-1}$ (constant) by using the parameters given by Mönch:[2,3] $A_X=0.86$ eV/Miedema-unit, $S_X=0.29$ eV/Miedema-unit; for the effective dipole length at the interface we have assumed the value of $\delta_i/\epsilon_i=2$ Å typical for wide band gap semiconductors.

The result of Eq. (3) is in very good agreement with the experiment: $\Phi_{Bn}-\Phi_{exp}(N)=0.28$ eV.

An interesting question remains to be answered, namely why the Schottky-barrier heights on Ga(0001) (Fig. 1, filled circles) for all metals, including Pt, lie close to the MIGS-model curve (full line in Fig. 1). Even though polarization induced charges had to be taken into account in the charge balance in Eq. (1), there is a negligible effect on the barrier height. A qualitative explanation might be, that reconstruction models of GaN(0001)[7] suggest the presence of a metallic Ga double layer which might effectively screen the polarization induced interface charge Q_{pol} and the refined MIGS model of Mönch[2,3] holds as is seen in the experimental results (Fig. 1).

In conclusion, our interpretation of the experimental Schottky-barrier height data on Pt/GaN is based on the contribution of spontaneous polarization charges to the interface charge balance. It gives a quantitative understanding of the experimental data for N-face polarity.[1] Our interpretation is in accordance with the picture of Schottky-barriers being determined by MIGS.

[1] U. Karrer, O. Ambacher, and M. Stutzmann, Appl. Phys. Lett. **77**, 2012 (2000).
[2] W. Mönch, Rep. Prog. Phys. **53**, 221 (1990).
[3] W. Mönch, J. Vac. Sci. Technol. B **17**, 1867 (1999).
[4] V. Heine, Phys. Rev. **138**, A1689 (1965).
[5] J. Tersoff, Phys. Rev. Lett. **52**, 465 (1984); J. Tersoff, Phys. Rev. B **32**, 6968 (1985); J. Tersoff, Surf. Sci. **168**, 275 (1986); J. Tersoff, Phys. Rev. Lett. **56**, 2755 (1986).
[6] F. Bernardini, V. Fiorentini, and D. Vanderbilt, Phys. Rev. B **56**, R10024 (1997).
[7] A. R. Smith, R. F. Feenstra, D. W. Greve, M. S. Shin, M. Skowronski, J. Neugebauer, and J. E. Northrup, J. Vac. Sci. Technol. B **16**, 2242 (1998).