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Temperature-dependent Kelvin probe measurements of band bending in *p*-type GaN

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The band bending in a Mg-doped, *p*-type GaN film grown by hydride vapor phase epitaxy was studied at various temperatures. At 295 K, the band bending in dark was calculated to be approximately −1.5 eV. However, when the sample was heated to 600 K for 1 h in dark before performing a measurement at 295 K, the calculated value of band bending in dark became about −2.0 eV. These results are explained by the fact that increasing the sample temperature exponentially increases the rate at which the band bending restores and allows for a more accurate value of band bending to be measured. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4747203]

Characterizing the surface of GaN films is of paramount importance, since surface conditions influence device performance. It is known that the surfaces of *n*- and *p*-type GaN commonly exhibit upward and downward band bending as a result of excess negative or positive surface charge, respectively. The exact source of this charge is still unknown.[1] The band bending and related depletion region have detrimental effects on the optical and electrical properties of GaN-based devices.[2] We consider two potential sources of surface charge: internal and external. Possible internal sources of surface charge include semiconductor surface states due to dangling bonds, reconstruction, structural and point defects, spontaneous polarization, or impurities. External sources of surface charge can include a surface oxide layer or adsorbed species. It has been established that a monolayer of chemisorbed oxygen exists on the surface of GaN, which may form a thin (∼1 nm) surface oxide.[3] The values of the upward band bending reported for *n*-type GaN are approximately 1 eV and do not vary much between reports.[4–7] However, the reported values of band bending for *p*-type GaN vary widely from about −0.8 to −3.0 eV.[8–13] The reason for such a wide range of band bending values in *p*-type GaN has, to date, not been given much consideration.

In the literature, there are few studies in which the sample temperature was varied while performing x-ray photoelectron spectroscopy (XPS) or ultraviolet photoelectron spectroscopy (UPS) measurements. The peak positions from XPS and UPS can be used to measure the near-surface band bending. However, the drawback is that the incoming x-rays generate a surface photovoltage (SPV) and reduce the band bending.[13] We believe that the temperature at which the measurements were taken affects the measured values of band bending calculated from these reports. Tracy *et al.*[8] measured the band bending in *p*-type GaN using XPS and UPS. In these measurements, the sample was annealed at 1140 K for 15 min and then, the temperature was reduced to 295 K before taking data. The calculated downward band bending in their sample was about −0.8 eV.

To minimize the effect of the SPV in XPS measurements, it is necessary to increase the sample temperature. Long and Bermudez[13] performed a temperature-dependent study of *p*-type GaN using XPS and UPS. Although the authors did not explicitly estimate the band bending, it can be calculated using the surface Fermi-level position and free carrier concentration. When the temperature was increased from 300 to 700 K, the magnitude of the calculated band bending increased from 0.77 to 2.15 eV for *p*-type GaN which can be attributed, at least partially, to the reduction of the SPV magnitude with increasing temperature. We have estimated that a typical x-ray intensity[13] on the order of $10^{14}\,\text{cm}^{-2}\text{s}^{-1}$ would produce an SPV signal of at least 0.2 eV. In comparison to XPS, Kelvin probe measurements of the surface potential are expected to be more reliable, since these measurements in dark do not affect the measured value of band bending. From surface potential data and the concentration of free holes reported by Eyckeler *et al.*,[12] we calculated the band bending in their *p*-type GaN sample to be about −3.0 eV. In their experiment, the sample was heated to about 1100 K in dark, before measurements with a Kelvin probe were performed at 150 K.

In this work, we studied the effect of temperature on SPV in *p*-type GaN in an effort to explain the disparity of band bending values reported in the literature. The SPV technique can be used to estimate the band bending in semiconductors. Illumination with band-to-band light generates electron-hole pairs in the depletion region that are separated due to the strong electric field. In *p*-type materials, band-to-band illumination causes photo-generated electrons to accumulate at the surface which reduces the net positive charge and therefore decreases the band bending. We have previously shown that the surface potential can be measured by the contactless Kelvin probe method, and that the band bending can then be estimated from SPV measurements and the dark contact potential difference (CPD) signal.[14–16]

We investigated several *p*-type GaN samples grown by hydride vapor phase epitaxy (HVPE), metal-organic vapor phase deposition (MOCVD), and molecular beam epitaxy (MBE). The sample which was studied extensively is a Mg-doped GaN film, with a thickness of about 3 μm, which was grown on *c*-plane sapphire by HVPE at TDI, Inc.[17] The

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concentration of uncompensated shallow acceptors (N_A – N_D) for this sample was estimated from capacitance-voltage measurements to be about $6.5 \times 10^{18}\,\mathrm{cm}^{-3}$. Ohmic contacts were formed by depositing Ni/Au layers around the sample periphery. The Hall effect data were ambiguous, most likely due to the existence of a thin, degenerate *n*-type layer near the GaN/sapphire interface.[18] However, the sample exhibited *p*-type conductivity from SPV and hot probe measurements. Assuming a compensation ratio of 0.5, we estimate that $N_A = 1.3 \times 10^{19}\,\mathrm{cm}^{-3}$ and $N_D = 6.5 \times 10^{18}\,\mathrm{cm}^{-3}$, which provides a concentration of free holes of $p = 7 \times 10^{15}\,\mathrm{cm}^{-3}$ at 295 K, if the ionization energy of the acceptor $E_A = 0.18$ eV. To account for errors in these estimates, we additionally analyzed the dependence of the Fermi-level position on the compensation ratio, which was varied from 0.2 to 0.8. At most, the Fermi-level position changed by ±0.04 eV within the range of temperatures used in this work and, therefore, does not introduce any significant error in our estimates of band bending.

The surface potential was measured using a Kelvin probe mounted inside an optical cryostat with a base pressure of about 10^{-6} mbar. Prior to illumination, the sample was allowed to restore in two different ways: stored in dark for at least 1 day at 295 K or heated to 600 K for 1 h. In both cases, the sample was illuminated from the front side using a HeCd laser (325 nm). The laser beam was passed through a window in the cryostat, and then through a perforated 4 mm diameter probe before reaching the sample surface. The maximum light intensity incident on the sample surface was ~40 mW/cm^2 and could be attenuated by about 10 orders of magnitude with a series of neutral density filters.

To estimate the near-surface band bending in dark, Φ_0, the SPV behavior can be fit using a thermionic model.[14] The SPV value, y_0, generated at a given excitation intensity, P_0, can be used to estimate Φ_0 in *p*-type GaN with the relation

$$y_0 = -\eta kT \ln\left(\frac{cP_0}{R_0} + 1\right) \qquad (1)$$

with

$$R_0 = s_p N_V \exp\left(\frac{\Phi_0 + (E_V - F)}{\eta kT}\right), \qquad (2)$$

where η is an ideality factor (expected to be close to one), k is Boltzmann's constant, T is the temperature, c is a geometrical factor that accounts for the portion of photons that are absorbed in the depletion region, R_0 is the rate at which holes move from the bulk to surface per unit time per unit area, s_p is the surface recombination velocity for holes, N_v is the effective density of states in the valence band, and E_v and F are the positions of the valence band maximum and Fermi level, respectively. Because the value of cP_0/R_0 in Eq. (1) is much greater than one for the range of light intensities used in this study, Eqs. (1) and (2) simplify to

$$y_0 \approx \Phi_0 - (F - E_v) + \eta kT \ln\left(\frac{s_p N_v}{cP_0}\right). \qquad (3)$$

This expression can be used to find Φ_0 if the other parameters are known. In our experiment, P_0 was calculated from the laser power density, and the parameter c was estimated to be 0.13 for front-side illumination of GaN with a calculated depletion region width of 12 nm. The value of (F-E_v) was estimated to vary from 0.20 to 0.23 eV with increasing temperature from 295 to 650 K for the studied HVPE-grown GaN sample. We assumed that s_p for GaN lies within the range of 10^3–10^7 cm/s with the most probable value of 10^5 cm/s.[19] Note that changing the value of s_p by four orders of magnitude introduces an error in the estimate of band bending of only ±0.2 eV. Finally, the temperature dependence of N_v has a negligible effect on y_0 because of its logarithmic dependence. Thus, it is expected from Eq. (3) that the magnitude of the SPV should *decrease* almost linearly with increasing temperature.

To examine the effect of sample temperature on the SPV generated in *p*-type GaN, the surface was illuminated for 1 s with $P_0 = 7 \times 10^{16}\,\mathrm{cm}^{-2}\mathrm{s}^{-1}$ at temperatures from 295 to 500 K. The SPV as a function of sample temperature is shown in Fig. 1, for the case when the sample was not pre-heated (empty circles) before the measurement, and for the case when it was pre-heated at 600 K in dark for 1 h before the measurement (filled circles). Note that at 295 K, the absolute value of the SPV for the sample with pre-heating is significantly larger than for the sample without pre-heating (see arrow in Fig. 1). Interestingly, when the sample was not pre-heated, the magnitude of the SPV *increased* from 0.55 to 0.8 eV as the temperature increased from 295 to 500 K. This behavior contradicts the thermionic model [Eq. (3)] which predicts that the magnitude of the SPV should decrease with increasing sample temperature. However, when the same sample was pre-heated at 600 K for 1 h before performing a measurement, the magnitude of the SPV *decreased* from 1.2 to 0.8 eV as the temperature increased from 295 to 500 K. Such a large value of SPV (−1.2 eV) observed after pre-heating indicates that the magnitude of Φ_0 apparently exceeds 1.2 eV at 295 K, whereas the estimated lower bound of $|\Phi_0|$ for the sample without preheating is only 0.55 eV.

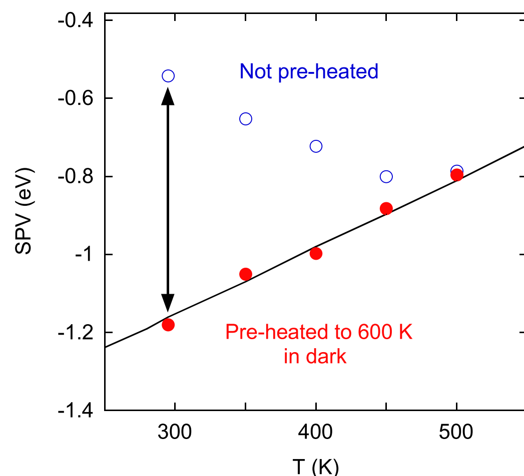

FIG. 1. SPV generated with $P_0 = 7 \times 10^{16}\,\mathrm{cm}^{-2}\mathrm{s}^{-1}$ as a function of sample temperature. Sample was pre-heated in dark at 600 K for 1 h (filled circles) or was not pre-heated (empty circles). The solid line is calculated using Eq. (3) with the following parameters: $c = 0.13$, $\eta = 1$, $\Phi_0 = -1.45$ eV, and $s_p = 10^5$ cm/s. To find the temperature dependence of F in Eq. (3), we used the following parameters: $N_A = 1.3 \times 10^{19}\,\mathrm{cm}^{-3}$, $N_D = 6.5 \times 10^{18}\,\mathrm{cm}^{-3}$, and $E_A = 0.18$ eV.

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The process of pre-heating the sample at high temperatures increases the rate of restoration for the band bending in dark, thereby providing more accurate values for subsequent SPV measurements. Therefore, the sample temperature is important when estimating the band bending in dark.

In order to estimate Φ_0, we fit the data in Fig. 1 by Eq. (3) with $\eta = 1$ (solid line), where Φ_0 is the only fitting parameter. With this method, the band bending in dark for the p-type GaN sample, after being pre-heated, is found to be -1.45 eV. We consider the magnitude of 1.45 eV as the lower bound for $|\Phi_0|$ because η varies between 1.3 and 3.1 in p-type GaN, according to the excitation intensity and temperature dependencies to be discussed later. These large values of η greatly affect the value of Φ_0 obtained from Eq. (3). Conversely, the value of η for n-type GaN is equal to one for a wide range of temperatures, and Φ_0 can be reliably and accurately determined from SPV measurements.[20] However, η is much larger than one for p-type GaN, and the above estimates may not be accurate and should be regarded with caution. An alternative method to estimate the band bending using Kelvin probe measurements is described below.

The band bending in dark can also be determined from the dark CPD signal using the expression

$$\Phi_0 = \phi_M - \chi - (E_g + E_V - F) - qV_{CPD}, \tag{4}$$

where χ is the electron affinity for GaN (3.2 eV),[21] E_g is the band gap width (3.43 eV at 295 K), and qV_{CPD} is the measured CPD multiplied by the electron charge. The work function of the stainless steel probe, $\phi_{M,}$ was estimated to be 4.8 eV from the measurement of a gold foil and 4.45 eV from data for an n-type GaN sample with $\Phi_0 = 1.05$ eV.[20] The latter was considered as a more reliable value, because the band bending in this sample was accurately established from the SPV measurements by using the thermionic model. Figure 2 shows the values of band bending determined from CPD data for several samples at temperatures between 295 and 500 K. These measurements were taken after the samples were pre-heated at 600 K which allowed the band bending to restore more fully. In addition to the HVPE sample, the data for two other p-type GaN samples grown by MBE and MOCVD and an n-type GaN sample grown by HVPE are shown for comparison. The CPD signal for all of these samples was obtained in a similar manner. The calculated band bending for all samples is independent of temperature and equals about +1 eV for the n-type sample and about -2 eV for all p-type GaN samples. Without preheating the sample, the calculated value of Φ_0 for the n-type GaN sample does not change, whereas for the p-type samples, the calculated absolute value of the band bending was typically smaller by about 0.3 eV than the values from experiments with preheating at 600 K. Note that the preheating can in principle affect the work function of the probe, and other errors in the parameters may propagate in the calculation. While the agreement between the results obtained from the SPV and CPD data is qualitative rather than quantitative for p-type GaN, both methods indicate that the large band bending cannot fully restore in dark at room temperature and, consequently, is underestimated.

To further investigate how temperature affects the dark value of band bending, the restoration of the SPV after illumination was measured at temperatures from 295 to 500 K. After illumination of the sample has ceased, the band bending is expected to restore to its dark value with a rate proportional to the sample temperature. The restorations of the SPV after short (1 s) UV illuminations at different temperatures are shown in Fig. 3. The amount of time required for the band bending to fully restore in dark has a strong dependence on temperature and can be fit by a thermionic model[14]

$$y(t) \approx y_0 + \eta kT \ln\left(1 + \frac{t}{\tau}\right) \tag{5}$$

with

$$\tau = \frac{\eta kT}{R_0}\frac{p_s(0)}{2\Phi_0}\exp\left(\frac{y_0}{\eta kT}\right), \tag{6}$$

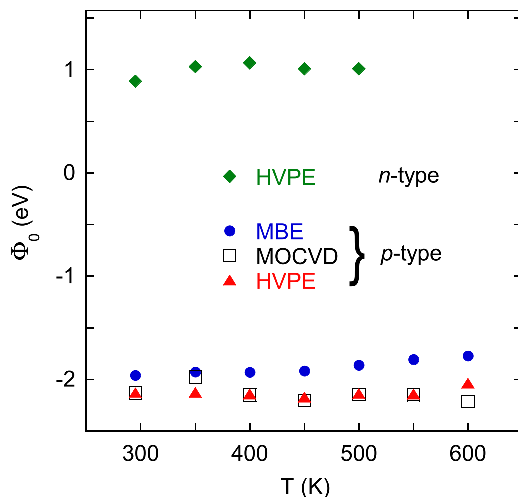

FIG. 2. Band bending in dark for both n- and p-type GaN calculated from CPD measurements in dark using Eq. (4) for p-type and using Eq. (31) from Ref. 14 for n-type. The data were obtained after pre-heating the sample for 1 h at 600 K in dark before each measurement.

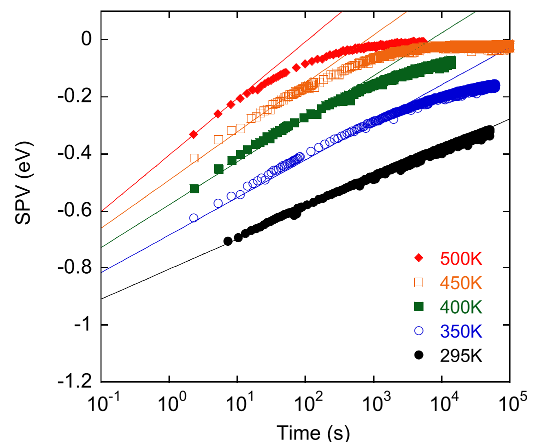

FIG. 3. Restorations of SPV after short (1 s) UV illuminations at $P_0 = 7 \times 10^{16}\,\mathrm{cm^{-2}s^{-1}}$ for temperatures from 295 to 500 K. Each measurement is taken after preheating the sample at 600 K for 1 h. The fits are calculated using Eq. (5) with $\tau = 0.001$ s and $y_0 = -1.12$, -1.08, -1.03, -1.0, and -0.9 eV; $\eta = 1.8$, 1.9, 1.9, 1.9, and 2; for $T = 295$, 350, 400, 450, and 500 K, respectively.

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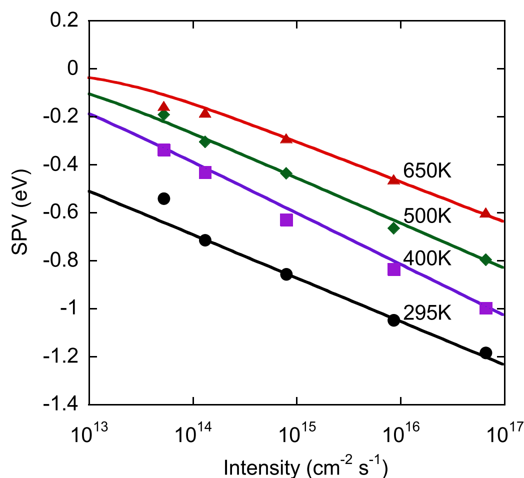

FIG. 4. Intensity-dependent SPV data taken at the indicated temperatures after preheating at 600 K for 1 h in dark. The solid lines are calculated using Eq. (1) with parameters: $c = 0.13$; $\eta = 3.1$, 2.7, 1.9, and 1.3; $R_0 = 2\times10^9$, 2×10^{11}, 5×10^{11}, and $2\times10^{12}\,cm^{-2}\,s^{-1}$ for $T = 295$, 400, 500, 650 K, respectively.

where y_0 is the SPV when illumination has ceased, t is the time elapsed after illumination, τ is a characteristic time delay which exponentially depends on the near-surface barrier, and $p_s(0)$ is the net density of positively charged states at the surface. Equation (5) is a simplified version of the restoration equation from a previous work that does not account for the complete restoration of band bending.[14] This equation is only meant to predict the behavior at the beginning of restoration and the slope. For this reason, there is no asymptotic behavior in the fits when the SPV data show complete restoration. As expected, the fits to the SPV data using Eq. (5) indicate that the initial slope of the restoration is faster at higher temperatures. By extrapolating the fit for 295 K, the SPV is predicted to fully restore in approximately 10^8 s (a few years). This takes four orders of magnitude more time than the complete restoration of the band bending at 500 K, which should occur in about 10^4 s (3 h). From these restoration rates, it is clear that heating the sample in darkness allows band bending values larger than 1 eV to fully restore, thereby providing more accurate baselines for SPV and CPD measurements.

Figure 4 shows the SPV as a function of excitation intensity at various temperatures for the HVPE p-type GaN sample after pre-heating. As predicted by Eq. (3), the magnitude of the SPV at any given excitation intensity decreases with increasing temperature, and the magnitude of the SPV increases logarithmically with excitation intensity at all temperatures. However, the slope of the SPV signal versus illumination intensity for temperatures from 295 to 650 K is larger than expected: η ranges from 3.1 to 1.3, respectively. The slope of the SPV dependence on light intensity begins to approach the predicted value at high temperatures, with $\eta = 1.3$ at 650 K. The dependence of η on T may indicate that the high resistivity of our p-type GaN sample is affecting the Kelvin probe SPV measurements. At higher temperatures, the sample conductivity greatly increases, and any effect due to the high resistivity of the sample should decrease. The larger than expected slope at low temperatures may be related to the Dember potential which arises due to the different mobilities of electrons and holes in GaN.[1] These measurements also indicate that the band bending values obtained at higher temperatures are more reliable.

In conclusion, we have observed that the temperature at which p-type GaN samples are kept in dark can, at least partially, explain the wide range of band bending values reported in the literature. Measurements performed at higher temperatures allow for the band bending to more fully restore and therefore provide larger and more accurate values of band bending in dark. If the measurements are performed at 295 K without pre-heating, however, then the band bending will not have sufficient time to fully restore and a "practical" value of band bending in dark of about −1.5 eV will be measured. It appears that the actual downward band bending is about −2.0 eV. This value was calculated from the dark CPD signal and is in agreement with the values estimated from fitting the SPV data with a thermionic model.

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