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Surface band bending of *a*-plane GaN studied by scanning Kelvin probe microscopy

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We report the value of surface band bending for undoped, *a*-plane GaN layers grown on *r*-plane sapphire by metalorganic vapor phase epitaxy. The surface potential was measured directly by ambient scanning Kelvin probe microscopy. The upward surface band bending of GaN films grown in the $[11\bar{2}0]$ direction was found to be 1.1 ± 0.1 V. Because polarization effects are not present on *a*-plane GaN, we attribute such band bending to the presence of charged surface states. We have modeled the surface band bending assuming a localized level of surface states in the band gap on the surface. It should be noted that the band bending observed for *a*-plane Iayers is comparable to that obtained on polar *c*-plane layers, and both *a*-plane and *c*-plane GaN films with similar surface treatments demonstrate comparable band bending behavior, indicating that charged surface states dominate band banding in both cases. © 2006 American Institute of Physics. [DOI: 10.1063/1.2188589]

Understanding of the prevailing mechanism which is responsible for the relatively high surface band bending observed on GaN surfaces plays an important role in achieving controllable surfaces and interfaces for GaN-based devices. Wurtzite GaN films grown along the [0001] direction, i.e., c-plane films, have polar surfaces with spontaneous polarization of -0.029 Cm⁻²,¹ which induces a surface charge density from 10^{13} to 10^{14} cm⁻². This spontaneous polarization induces a large negative surface charge for Ga-polar films and a positive charge for N-polar films,² but the resultant surface band bending is also affected by charged dopants, defects, adsorbates, and surface states. In fact, measured differences of band bending between the polarities vary significantly from 1.4 eV by photoemission spectroscopy,³ to values ranging from 0.6 eV to 0.1 eV by ambient scanning Kelvin probe microscopy (SKPM).⁴⁻⁶ It has also been shown that different surface treatments, such as cleaning, etching, annealing, and passivation, result in different effects on the observed surface band bending.^{4,5,7–11} To investigate the relative importance of the polarization charge with respect to surface band bending, it is therefore useful to examine *a*-plane GaN films grown along the $[11\overline{2}0]$ direction, which are nonpolar and have no polarization-induced surface charges.

The *a*-plane GaN films used in this study were grown on $(1\overline{1}02)$ *r*-plane sapphire (±2° tolerance). The sapphire substrates were first annealed at 1400 °C for 1 h in air to remove surface damage and obtain atomically smooth surfaces. The GaN films were then grown in a low-pressure organometallic vapor phase epitaxy system using trimethyl-gallium and ammonia for Ga and N sources, respectively. Following *in situ* annealing, a 45 nm thick GaN buffer layer was deposited at 550 °C. Both samples studied in this work had a sandwich structure with an upper layer grown under the same conditions, but with intermediate layers grown with different III-V ratios and a temperature difference

of ~100 °C. The total GaN film thickness was ~3 μ m and growth temperatures were from 970 to 1070 °C. Samples were unintentionally doped with a carrier concentration of ~10¹⁶ cm⁻³, corresponding to a Fermi level 0.14 eV below the conduction band. The crystalline orientation of the GaN films was determined using a 2θ x-ray diffraction scan (λ =1.541 Å). The sapphire (2204) and GaN(1120) peaks of one sample are shown in Fig. 1. The full width at half maximum is 0.2°, showing good crystalline quality and consistent with previously reported results.¹²

SKPM was used to measure the contact potential difference $(V_{\rm cp})$ between the GaN surface and a gold-coated tip. The surface band bending (Φ) was calculated using the formula

$$\Phi = \phi_M - qV_{\rm cp} + \Phi_{\rm off} - \chi + E_F, \tag{1}$$

where ϕ_M is the tip metal work function $(\phi_M = 5.1 \text{ eV for Au})$, χ is the electron affinity $(\chi = 3.2 \text{ eV for GaN})^8$ and E_F is the Fermi level with respect to the conduction band minimum. Φ_{off} is the measured offset determined by measuring V_{cp} on a gold film calibration sample.^{13,14} SKPM measurements were acquired for air-exposed samples and then re-



FIG. 1. 2θ scan of sample shown in Fig. 2(a), where the sapphire $(2\overline{2}04)$ and GaN $(11\overline{2}0)$ peaks verify the growth surface as *a*-plane GaN.

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FIG. 2. (a) and (c) AFM topography images, and (b) and (d) corresponding surface potential images of two different air-exposed *a*-plane GaN films. Image sizes are $5 \times 2.5 \ \mu m^2$ and height variations are: (a) Δz =60 nm, (b) ΔV =110 mV, (c) Δz =200 nm, and (d) ΔV =150 mV.

taken after degreasing (acetone, methanol, deionized water) and chemical etching in boiling HCl:HNO₃. To investigate the variation of band bending under ultraviolet (UV) illumination, i.e., the surface photovoltage, a pulsed nitrogen laser was used with photon energy of 3.68 eV.

Figure 2 shows the atomic force microscope (AFM) topography and corresponding SKPM surface potential images of two *a*-plane GaN samples. For one of the samples [Figs. 2(c) and 2(d), there is some correlation between the topography and SKPM images, most likely because the sample topography is more rough ($\Delta z = 200$ nm). The average surface potential for both samples is 0.7±0.1 V, which corresponds to an upward surface band bending of 1.1 ± 0.1 eV. This value did not change after cleaning in HCl: HNO₃. The band bending for a-plane samples, as well as the effect of cleaning, is comparable to that obtained for polar *c*-plane samples grown both by molecular-beam epitaxy and metalorganic chemical vapor deposition.^{5,11} The surface band bending of the *a*-plane samples decreased by 0.1 to 0.2 eV under UV illumination and had a recovery time of a few seconds. This behavior is also similar to that observed for c-plane samples previously studied by this group.^{5,13} Given that both *a*-plane and *c*-plane GaN films with similar surface treatments demonstrate comparable band bending behavior, it appears that surface states play a predominant role in band bending.

The upward band bending at the surface of *a*-plane GaN is consistent with the presence of charged acceptorlike surface states. While the detailed nature of such surface states requires additional study, the band bending can be explained using the model described by Mönch.¹⁵ The total charge at the surface Q_1 and in the space-charge region Q_2 can be expressed as

$$Q_{1} = \frac{-qN}{\exp\left[\frac{E_{ss} - E_{F}}{kT}\right] + 1},$$

$$Q_{2} = \sqrt{2\epsilon_{b}\epsilon_{0}nkT\left[\exp\left(\frac{-|\Phi|}{kT}\right) + \left(\frac{|\Phi|}{kT}\right) - 1\right]},$$
(2)
(3)

where N is the areal concentration of surface acceptors with energy E_{ss} , ϵ_b is the bulk dielectric constant, n is the bulk



FIG. 3. Calculated dependence of the surface band bending Φ on the density of surface states for two localized acceptor levels, which are located at 1.2 eV or 1.6 eV below the conduction band at the surface (solid lines). The experimentally obtained value of surface band bending is shown as the dotted line.

carrier concentration, and Φ is the surface band bending. Assuming charge neutrality, i.e., $Q_1+Q_2=0$, Fig. 3 shows the calculated band bending as a function of the concentration of surface acceptors for two different acceptor energy levels. When the Fermi level is close to the surface state energy, the band bending Φ becomes almost constant with respect to surface state density, indicating the condition of Fermi level "pinning."

As shown in Fig. 3, the saturation band bending value was calculated to be 1.1 eV for a surface state acceptor level located 1.2 eV below the conduction band at the surface. The saturation band bending increases to 1.5 eV in the case of an acceptor level with energy 1.6 eV. The experimentally obtained band bending value of $\Phi=1.1 \text{ eV}$ can therefore be modeled as a single acceptor level with a range of possible energy values and surface state densities (see crossing of dotted line with calculated lines in Fig. 3). The band bending is consistent with an acceptor level at 1.2 eV having a surface state density of 2×10^{12} cm⁻², or with a level at 1.6 eV having a density of only 3×10^{11} cm⁻². In reality, both acceptor and donor type surface states may be present and their distribution would be more complicated than assumed here. The density of states used here is therefore considered to be an effective density of surface acceptors.

We have measured surface band bending of 1.1 ± 0.1 eV for *a*-plane GaN films using ambient SKPM. The band bending obtained for nonpolar *a*-plane layers is similar to previously reported values for air-exposed polar *c*-plane layers, and both types of GaN films with similar surface treatments demonstrate comparable band bending behavior. Because polarization charges are not present on nonpolar, *a*-plane GaN, we attribute the surface band bending to charged surface states. These states can be the same nature and dominant for both crystalline surfaces. The distribution and density of these surface states determine the band bending, where the surface state density for a given value of band bending can vary significantly for different localized energy levels.

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