Surface states and origin of the Fermi level pinning on non-polar GaN $(1\bar{1}00)$ surfaces

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GaN $(1\bar{1}00)$ cleavage surfaces were investigated by cross-sectional scanning tunneling microscopy and spectroscopy. It is found that both the N and Ga derived intrinsic dangling bond surface states are outside of the fundamental band gap. Their band edges are both located at the $\bar{\Gamma}$ point of the surface Brillouin zone. The observed Fermi level pinning 1.0 eV below the conduction band edge is attributed to the high step density but not to intrinsic surface states.

Group-III nitrides raised considerable attraction for green, blue, and ultraviolet laser and light emitting devices. Therefore, intensive efforts have been invested to improve the quality of the epitaxial growth. One particular challenge is the position of the Fermi level at the growth surface. For the presently used polar GaN(0001) growth surface, surface states were identified as origin of the Fermi level pinning. In contrast, for the non-polar GaN surfaces only little is known about the positions of the surface states and thus their possible influence on the Fermi energy. This is due to the lack of experimental data and disagreements between the existing theoretical calculations. This lack of understanding is particularly embarrassing in the light that the growth along non-polar GaN directions is very appealing, due to the absence of electric fields caused by piezoelectricity and spontaneous polarization. Therefore, we investigated non-polar n-type GaN$(1\bar{1}00)$ cleavage surfaces by scanning tunneling microscopy (STM) and spectroscopy (STS) [1]. We identify that no filled N or empty Ga derived dangling bond surface states are present within the fundamental band gap. The only spectroscopic feature within the band gap arises from electrons accumulated in defect states, pinning the Fermi energy at about 1 eV below the conduction band minimum.

Figure 1a illustrates the typical morphology of the GaN$(1\bar{1}00)$ cleavage surface, which consists of atomically flat terraces separated by monoatomic steps. On terraces we measured the current-voltage spectra at different tip-sample separations (Fig. 1b). In order to identify the origins of the tunnel current and thus the positions of the band edges relative to the Fermi energy E_F, we turn to the logarithmic display of the current I and the normalized differential conductivity $(\mathrm{d}I/\mathrm{d}V)/(\overline{I/V})$ as a function of the sample voltage (Fig. 2). The logarithmically displayed current curve in Fig. 2a exhibits (i) a clear onset at +1.0 V of the tunnel current into the empty conduction band states of the surface (I_C) and (ii) two different current contributions at negative voltages, i.e. I_{acc} at voltages between 0 and –2.5 V and $I_V + I_{acc}$ at voltages V < -2.5 V. The current contribution I_{acc} is located at energies within the band gap of GaN.

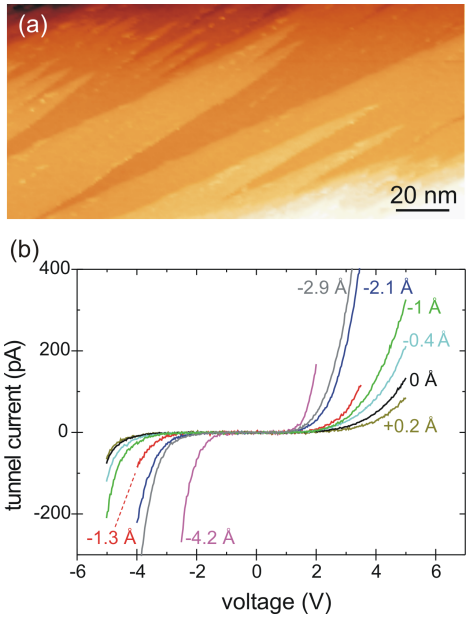

FIG. 1: (a) Constant-current empty state STM image of a cleaved GaN$(1\bar{1}00)$ surface. (b) Current-voltage spectra measured on the flat terraces. The different curves correspond to different tip-sample separations $z = z_0 + \Delta z$ (Δz given at each curve and z_0 defined by a set voltage and current).

The different observed current contributions can be explained as follows [1]: (i) I_C arises from a direct tunneling into empty conduction band states. Thus, the onset voltage at +1.0 V corresponds to the position of the conduction band edge at the surface (E_C). This indicates a Fermi level pinning 1.0 eV below E_C. (ii) the currents (I_{acc}) arises from an accumulation of electrons in the empty defect band, which induces the observed pinning of the Fermi energy as illustrated in detail in Ref. [1]. Finally, (iii), if the magni-

tude of negative voltage is increased above the corresponding energy of the valence band edge E_V, also filled valence band states face empty tip states and additional electrons can tunnel yielding the I_V current contribution. This effect leads to a second onset of the tunnel current close to –2.5 V in Fig. 2a, which thus corresponds to the valence band edge of the GaN surface (E_V).

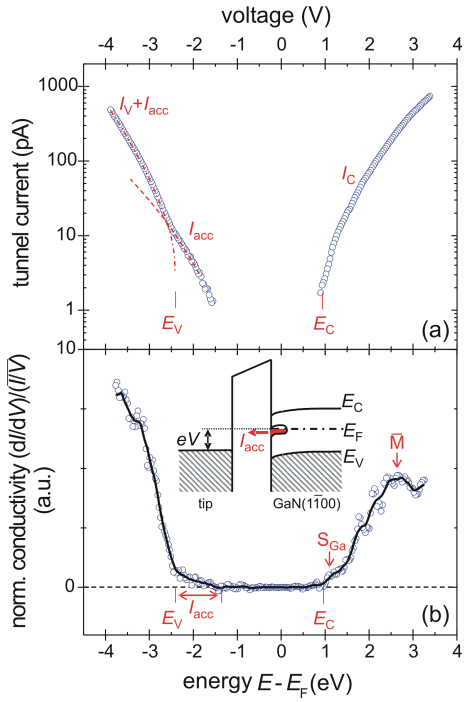

FIG. 2: (a) Logarithmic display of the tunnel current as a function of voltage. The conduction band (I_C), accumulation (I_{acc}), and valence band (I_V) currents are indicated. The positions of the valence and conduction band edges (E_V and E_C) are marked. (b) Normalized differential conductivity $(dI/dV)/(\overline{I/V})$. S_{Ga} marks the energetic minimum and $\bar{M}$ the maximum DOS of the empty Ga dangling bond surface state. The band onsets E_V and E_C and the effect of the accumulation current I_{acc} are clearly visible. Inset: Schematic of the origin of the accumulation current. Note, only the effect of the tip-induced band bending is shown.

The energetic positions of E_V and E_C can be seen even better in the normalized differential conductivity $(dI/dV)/(\overline{I/V})$ (Fig. 2b), which corresponds to the density of states (DOS). At E_F– 2.4 eV and at E_F + 1.0 eV clear onsets of the valence and conduction band DOS are visible, respectively. Thus, the band gap at the surface is (3.4±0.2) eV wide, matching well the bulk band gap of GaN, supporting our identification of the band edges. The minimum of the empty Ga dangling bond surface state (S_{Ga}) can be attributed to the shoulder 0.1-0.2 eV above E_C. The large peak at about E_F+2.5 eV ($\bar{M}$ in Fig. 2b) can also be related to the flat part of the empty dangling bond's band dispersion around the $\bar{M}$ point of the surface Brillouin zone, where the DOS is largest.

This can be further supported by an estimation of the momentum of the tunneling electrons through an analysis of the exponential decay of the tunnel current $I \sim e^{-2\kappa \cdot z}$ with increasing tip-sample separation z. Figure 3 shows the measured decay constant 2κ as a function of the voltage obtained for the largest tip-sample separations, where the effect of tip-sample interactions are negligible. The decay constant 2κ is approximately given by:

$$2\kappa = 2 \cdot \sqrt{\frac{2m_e}{\hbar^2}\left(B - \frac{|eV|}{2}\right) + |k_{||}|^2}$$

with $m_e$the electron mass and $k_{||}$ the parallel wave vector of the tunneling electrons. This approximation is shown as solid line in Fig. 3 for $k_{||}$ =0 and an estimated effective tunneling barrier B= 4.3 eV. At negative voltages and at small positive voltages (around 2 to 3 V) the measured values lie close to the calculated curve, indicating tunneling of electrons with $k_{||}$ =0. Thus, the N and Ga derived dangling bond surface states form a direct band gap at the $\bar{\Gamma}$ point. At larger positive voltages the decay constant is larger than expected for tunneling with $k_{||}$ =0. This indicates tunneling from the edge of the Brillouin zone, in agreement with the predicted dispersion of the empty surface state and the above interpretation of the peaks in the conduction band.

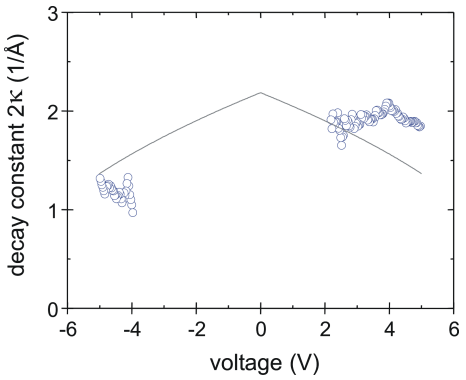

FIG. 3: Decay constant 2κ as a function of the voltage (open circles). The solid line shows the calculated trend for tunneling with zero parallel wave vector. These data reflect the dispersion of the surface states.

Finally, the filled DOS leading to I_{acc} is several orders of magnitude smaller than that of an accumulation zone in the conduction band. This is in good agreement with an origin of I_{acc} in pinning states, whose concentration is typically in the range of 10^{11} to 10^{13} cm^{-2}, i.e. much less than the DOS of the conduction band or of a dangling bond surface state. Thus, no intrinsic N and Ga derived dangling bond surface states are present in the fundamental band gap of GaN$(1\bar{1}00)$ surfaces and the observed Fermi level pinning cannot arise from the dangling bond surface states. Instead it can be attributed to the large step densities.

[1] L. Ivanova, S. Borisova, H. Eisele, M. Däne, A. Laubsch, and Ph. Ebert, Appl. Phys. Lett. **93**, 192110 (2008).