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Direct measurement of the band gap and Fermi level position at InN(11$\bar{2}$0)

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A nonpolar stoichiometric InN(11$\bar{2}$0) surface freshly cleaved inside UHV was investigated by scanning tunneling microscopy and spectroscopy. Due to the absence of intrinsic surface states in the band gap, scanning tunneling spectroscopy yields directly the fundamental bulk band gap of 0.7 ± 0.1 eV. The Fermi energy is pinned 0.3 eV below the conduction band minimum due to cleavage induced defect states. Thus, intrinsic electron accumulation can be excluded for this surface. Electron accumulation is rather an extrinsic effect due to surface contamination or material decomposition, but not an intrinsic material property of InN. © *2011 American Institute of Physics*. [doi:10.1063/1.3553022]

InN in principle opens up the possibility of using only one ternary III-V semiconductor alloy (InGaN) in optoelectronic devices to cover the whole visible spectral range.[1] Despite this, even basic material properties of InN are still under debate. Largely deviating fundamental band gap values were reported, ranging from ~2.0 to ~0.7 eV.[1–3] Furthermore, the intrinsic energetic position of the Fermi level is unclear, i.e., whether the Fermi level is located within the fundamental band gap or shifted into the conduction band. In the latter case an electron accumulation at the surfaces of the crystal is induced.[4] Such an electron accumulation is typically observed at InN surfaces,[5,6] raising the question of whether it is an intrinsic material property or not.

One of the major problems addressing these issues experimentally is the lack of combined structural and electronic measurements. This is particularly embarrassing because the interpretation of optical data requires knowledge of the structural properties. For an accurate optical band gap determination, it is important to use high quality material. Combining scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) enables simultaneous probing of structural and electronic material properties.[7] In addition, it allows a direct access to both empty and filled electronic densities of states.[8,9]

In order to probe bulk properties by STM and not only surface effects or contamination, a clean and stoichiometric surface is necessary. This can be achieved by cleaving InN along nonpolar planes[10,11] in UHV.[12] In our experiment we applied cross-sectional STM and STS at the nonpolar InN(11$\bar{2}$0) surface in order to obtain information about the structural and electronic properties as well as information about correlation effects between them. The experiments were performed using a 1.2 μm thick *n*-type InN(000$\bar{1}$) layer (carrier concentration $\sim 2 \times 10^{18}$ cm^{-3} and mobility of ~1600 cm^2/V s) grown on an ~80 nm thick AlN(000$\bar{1}$) buffer on a Si(111) substrate.[3] The samples were cleaved in ultrahigh vacuum along the (1$\bar{1}$0) plane of the Si substrate and therewith along the (11$\bar{2}$0) surface of the deposited wurtzite structure AlN and InN layers.[12,13] For the investigation a homebuilt scanning tunneling microscope with an SPM 1000 (RHK) control unit was used.

Figure 1(a) shows an overview STM image of the cross-sectional cleavage surface through the InN/AlN/Si layers. On the left side of the image the morphology of the Si(1$\bar{1}$0) cleavage surface is visible, consisting of {1$\bar{1}$1} oriented terraces. Their size is found to be about 15 nm, typical for Si(1$\bar{1}$0) surfaces.[14] The ~80 nm thick wurtzite AlN buffer layer appears extremely rough. Finally, InN at the right side exhibits a much smoother (11$\bar{2}$0) surface morphology consisting of small terraces with step separations of 2–5 nm [Fig. 1(b)].

This assignment of the InN layer and the Si substrate can be proven further by the different electronic properties as detected by STS at the respective areas [Fig. 1(c)]. The Si(1$\bar{1}$0) surface exhibits a metallic behavior in the current-

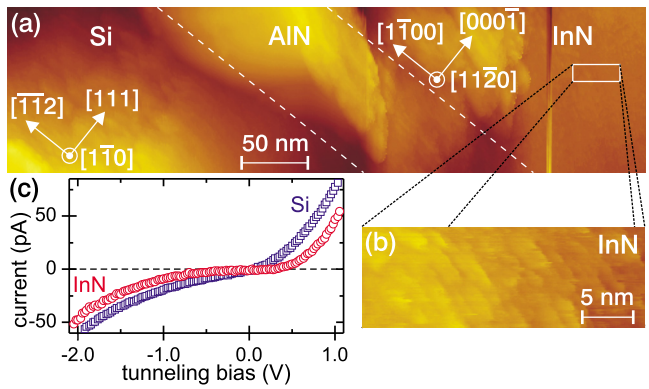

FIG. 1. (Color online) (a) Overview of constant-current STM image of the cross-sectional cleavage surface through the InN/AlN/Si layers measured at V_{set}=−1.5 V and I_{set}=35 pA. (b) Zoom-in STM image of the InN(11$\bar{2}$0) surface (V_{set}=−3.1 V and I_{set}=35 pA). (c) *I-V* curves measured on the metallic Si(1$\bar{1}$0) [squares] and semiconducting InN(11$\bar{2}$0) [circles] cleavage surfaces.

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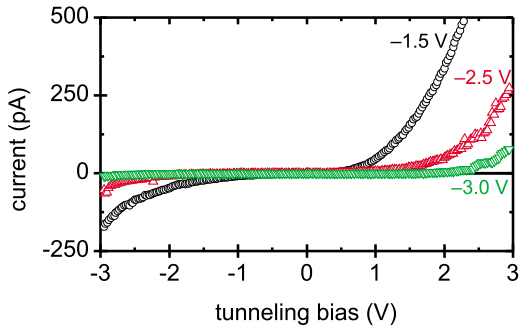

FIG. 2. (Color online) *I-V* curves measured on InN(11$\bar{2}$0) with different tip-sample separations, adjusted using different set voltages V_{set} as labeled and a set current I_{set}=35 pA.

voltage spectrum (*I-V* curve with nonzero slope) without any band gap [squares in Fig. 1(c)]. This is in agreement with previous measurements[14] and arises from intrinsic surface states within the fundamental band gap of Si(1$\bar{1}$0). In contrast, *I-V* curves measured at the InN layer exhibit a clear plateau with zero slope in the *I-V* curve [circles in Fig. 1(c)]. This demonstrates the presence of a band gap.

In order to analyze the fundamental intrinsic electronic material properties (band gap, energetic position of the Fermi level, Fermi level pinning, etc.) of InN in more detail, *I-V* curves were measured at different tip-sample separations (Fig. 2). The different tip-sample separations were adjusted using different set-point tunneling biases (V_{set}) and currents (I_{set}), before holding the tip at a certain position. At a constant I_{set} the tip-sample separation increases with $|V_{set}|$. Independent of the actual tip-sample separations all three *I-V* curves exhibit a bias range with no detectable current (detection limit of ~1 pA) around a tunneling bias of 0 V (Fig. 2). The absence of the current in principle indicates the presence of a band gap. However, the transmission coefficient for electron tunneling decreases with tip-sample separation. As a result the apparent band gap increases, and the band edge positions cannot be determined due to insufficient sensitivity of the current measurement.

Therefore, we concentrate in the following on a tip-sample separation on one hand being small enough for a sufficient sensitivity even within the band gap, but on the other hand being still well in the tunneling regime (no point contact). Figure 3(a) shows a magnified detail of the *I-V* curve with V_{set}=−1.5 V and I_{set}=35 pA. In order to identify the origins of the current and thus the energetic positions of the band edges relative to the Fermi energy (E_F), we first turn to the logarithmic display of the absolute current and the normalized differential conductivity $(dI/dV)/(\overline{I/V})$ as a function of the sample bias [Figs. 3(b) and 3(c), respectively]. The logarithmically displayed current curve in Fig. 3(b) exhibits (i) a clear single onset at +0.3 V of the tunneling current into the empty conduction band states of the surface (I_C) and (ii) two different current contributions at negative biases, i.e., $I_{acc,defect}$ at biases between V=−0.4 V and V=0 V and $I_V+I_{acc,defect}$ at biases $V<-0.4$ V. The current $I_{acc,defect}$ contributes already significantly at energies within the band gap of the InN. The different observed current contributions can be explained as follows:

First, at positive sample biases the tunneling current flows if the Fermi level of the tip is energetically above the conduction band edge of the surface. Thus, the onset bias at

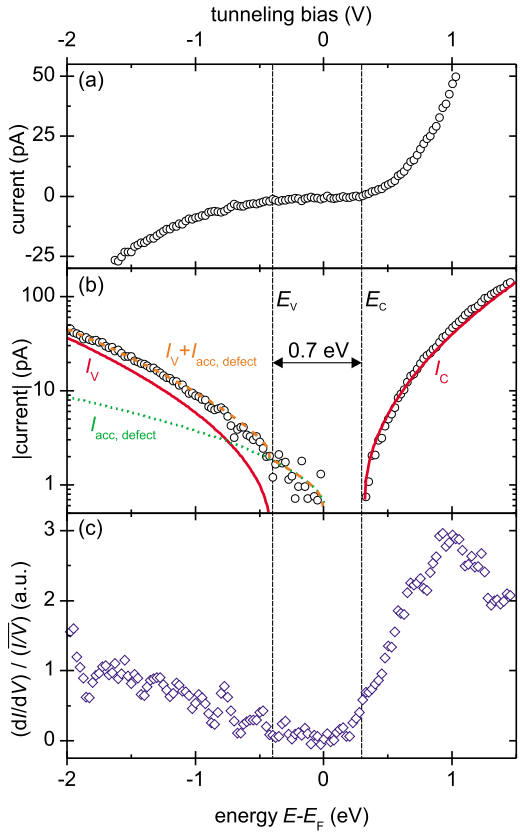

FIG. 3. (Color online) (a) Linear and (b) logarithmic displays of an *I-V* curve, and (c) normalized differential conductivity of InN(11$\bar{2}$0). In (b) the solid lines indicate the current contributions due to electrons tunneling into the conduction band (I_C) and out of the valence band (I_V). The dotted line shows the tunneling current due to extrinsic defect states in the band gap. The lines guide the eye.

+0.3 V corresponds to the position of the conduction band edge at the surface (E_C). This indicates a Fermi level pinning 0.3 eV *below* E_C.

Second, if the bias is decreased below the corresponding energy of the valence band edge (E_V), filled valence band states face empty tip states and electrons can tunnel, yielding the I_V current contribution. This effect leads to the intensive onset of the tunnel current close to a bias of −0.4 V in Fig. 3(b), corresponding to the valence band edge (E_V) of the InN surface.

Third, currents at tunneling biases corresponding to energies within the fundamental band gap of a semiconductor were already observed previously.[8,15–17] The observation of such currents requires filled semiconductor states to face empty tip states at biases corresponding to energies within the band gap. Such a situation can occur if (i) intrinsic surface states exist in the band gap, (ii) electrons accumulate at the InN surface, or (iii) defects are present at the surface. The $(dI/dV)/(\overline{I/V})$-curve in Fig. 3(c) exhibits neither intense peaks in the band gap nor metallic properties. Thus, intrinsic surface states within the band gap (i) can be ruled out. An electron accumulation at the surface requires the Fermi level to be above E_C. However, in our case, E_F is pinned 0.3 eV below E_C. Thus, $I_{acc,defect}$ cannot arise from a charge carrier accumulation zone in the conduction band (ii). Finally, our cleavage surface exhibits a high concentration of steps. At the step edges half filled defect states exist, leading to a pinning of the Fermi energy in the band gap, as observed.

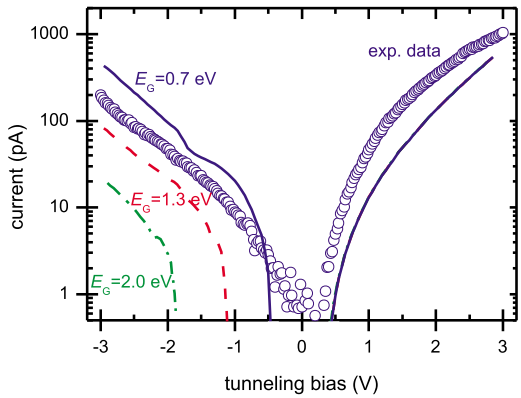

FIG. 4. (Color online) Comparison of the experimentally measured current with theoretically calculated ones for three different band gap values, as labeled. For the calculation a tip-sample separation of 0.85 nm and a tip work function of 4.5 eV were used.

The proximity of the biased tip results in a tip-induced local band bending, even if the Fermi level is pinned globally at the same time. Thereby, the defect state occupation can significantly change, and electrons accumulate in the defect state locally. Therefore, we attribute the current $I_{\mathrm{acc,defect}}$ to this effect.[16]

For further data evaluation we compare the measured current with calculations following Refs. 8, 15, and 18. For these calculations we assume an E_F pinning by defect states 0.3 eV below E_C, as observed experimentally (see above) and also indicated in Ref. 12. Figure 4 shows the calculated currents for three different band gaps, i.e., 2.0, 1.3, and 0.7 eV, together with the experimental data. The measured onsets of the current are best described by the calculation for a band gap E_G=0.7 eV, even if the absolute values of the calculated and measured currents are slightly different.

In our measurements on a clean and stoichiometric nonpolar InN$(11\bar{2}0)$ surface, we find a band gap of E_G =0.7 eV and the Fermi level to be located within this band gap. At this surface, steps and defects pin the Fermi level within the band gap. This shows that the intrinsic Fermi level (without doping and defects) is located within the band gap and not in the conduction band. Thus, the electron accumulation reported before for the InN$(11\bar{2}0)$ surface[5] is not an intrinsic property. Cleaving fresh surfaces in UHV, as performed here, yields contamination free stoichiometric surfaces. In contrast, as-grown surfaces may suffer from H_2 contamination. Upon air exposure, contamination by organics as well as O_2 and H_2O occurs. Aging effects of InN surfaces may cause nonstoichiometric InN surfaces with excess In due to the disappearance of N_2. Typically, In–In bonds cause occupied surface states above the conduction band minimum, and hence generate an electron accumulation layer.[11] For the unaged stoichiometric nonpolar InN$(11\bar{2}0)$ surface the absence of an electron accumulation layer was predicted[19] and is observed here. Thus, it can be concluded that electron accumulation at InN is not intrinsic, but primarily connected to nonstoichiometry and/or contaminations.

In conclusion, we prepared a fresh stoichiometric nonpolar InN$(11\bar{2}0)$ surface by cleaving inside UHV. Scanning tunneling spectroscopy yields a fundamental band gap of 0.7 ± 0.1 eV without intrinsic surface states. Defect states pin the Fermi energy 0.3 eV below the conduction band minimum. Due to the position of the Fermi level at the InN$(11\bar{2}0)$ surface within the fundamental bulk band gap intrinsic electron accumulation can be excluded for this surface. Electron accumulation is rather an extrinsic effect due to surface contamination or material decomposition, but not an intrinsic material property of InN. Thus, there is no intrinsic obstacle for *p*-type doping.[20]

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