A comparison of the valence band structure of a GaN single crystal and MOVPE grown thin films – an angle-resolved photoemission study

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Gallium nitride is one of the most promising materials for building blue laser diodes. Two different forms of GaN samples with the wurtzite crystal structure are available: single crystals grown under high pressure [1] and thin films grown using either MOVPE or MBE techniques. We were able to perform a comparative study on both types of samples under the same conditions. The single crystal GaN sample was produced in UNIPRESS Institute in Warsaw, but the sample dimensions were very small (around 0.2 mm thick, 4 mm² area) and cleaving in UHV along (0001) crystallographic direction was not possible. The MOVPE sample was made at Bremen University and grown on a sapphire substrate. The advantages of such samples are the larger sample area (5x5 mm²) and availability. Similar angle-resolved photoemission experiments have been carried out previously on cleaved GaN [4] and GaN samples grown by MBE [2]. A detailed theoretical analysis has been performed for the GaN (0001) surface by Strasser et. al. [3].

![Figure 1: Normal emission photoemission spectra for a single crystal (left) and the MOVPE (right) GaN sample recorded for photon energies between 14 and 29 eV.](image)

The measurements were performed at the SEYA F2.2 beamline at HASYLAB. This station is equipped with Seya-Namioka monochromator (5-40 eV energy range, 0.5 Å resolution) and angle-resolved electron...
spectrometer (40 meV resolution at 2 eV pass energy). The sample transfer system and UHV chambers permit a variety of sample preparation techniques. Exactly the same cleaning procedure was used for both samples; prolonged outgassing at 450 – 500 °C, then Ar ion sputtering at 0.5 kV, 25 mA for 30 min followed by annealing. Excellent, sharp LEED spots and no charging effects were observed for both samples, indicating very good surface crystallinity over the whole sample area. The high conductivity arises from the inherent doping of the samples.

Figure2: Angle resolved spectra for Γ-K direction in the Brillouin zone from single crystal GaN and the corresponding experimental band structure. The theoretical bulk and surface state bands calculated by Strasser et. al. [3] are indicated by squares and triangles.

The photoemission spectra show that sample cleaning process was highly effective. The excellent (5 · 10^-11 mbar or lower) ultra high vacuum in the analyser chamber allowed extended measurement periods of up to 24 hours cycles between cleaning cycles. Complete sets of photoemission spectra could be recorded within each measurement period. A normal-emission data set was always recorded first for Brillouin zone Γ-point determination followed by ARPES measurements for both sample orientations as determined from the LEED pattern.

There is a considerable similarity between the spectra from both materials. The band structures calculated from the angle-resolved spectra show quite good agreement with the theoretical calculations and presence of bands originating from surface states are observed in both types of samples.

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References