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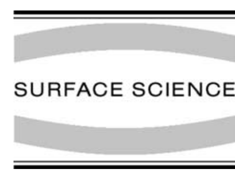
Surface Science 584 (2005) 169–178



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Angle-resolved photoemission from stoichiometric GaN(0001)-1 × 1

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Received 30 December 2004; accepted for publication 25 March 2005
Available online 14 April 2005

Abstract

We present results from an angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) investigation using synchrotron radiation of a stoichiometric Ga-polar GaN(0001)-1 × 1 sample grown by metal-organic chemical vapour deposition (MOCVD). The electronic structure of the surface was investigated with ARUPS along the $\overline{\Gamma}$–$\overline{K}$–$\overline{M}$, $\overline{\Gamma}$–$\overline{M}$, and Γ–A directions of the main symmetry lines of the surface and bulk Brillouin zones. We find one surface state close to the valence band maximum (VBM) at Γ, dispersing down and emerging into the projected band gap in the region around $\overline{K}$. From a comparison with a density functional theory (DFT) calculation [F.-H. Wang, P. Krüger, J. Pollmann, Phys. Rev. B 64 (2001) 035305-1], three additional surface related features are proposed, but no strongly dispersing Ga dangling bond band is observed. We find the VBM at 3.45 eV below the Fermi energy.
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Keywords: Angle-resolved photoemission; Low energy electron diffraction (LEED); Surface electronic phenomena; Surface reconstruction; GaN; Photoelectron spectroscopy; Synchrotron radiation; Ammonia; Semiconducting films

1. Introduction

The wide band gap semiconductor GaN has attracted a lot of interest due to its use in e.g. blue LED [1] of high brightness.

The bulk and surface electronic structures of GaN is thereby of large interest in order to fully control their properties and for the understanding of their behaviour during deposition of metal contacts and overlayers. We have developed a preparation method yielding well-ordered, stoichiometric surfaces with low amounts of surface contaminants. Detailed investigations of the electronic structure of this stoichiometric surface are, however, lacking. Most published results are from

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doi:10.1016/j.susc.2005.03.054

samples that have been cleaned by sputtering, which usually does not yield a stoichiometric surface, not even by the use of nitrogen (N) ions instead of argon (Ar) ions and subsequent annealing. Some examples from published results from wurtzite GaN samples are given below.

The surface and bulk electronic structures of a N-polar wurtzite GaN bulk crystals have been studied by Kowalski et al. [2,3]. They prepared clean surfaces with chemical polishing, sputtering with Ar and vacuum annealing.

Plucinski et al. [4] have published a comparative ARUPS study of the bulk and surface electronic structure of single crystals and thin films of GaN grown by metal-organic chemical vapour deposition (MOCVD) and metal-organic vapour phase epitaxy (MOVPE). Ar sputtering and vacuum annealing were used for all types of samples as the cleaning method.

Ding et al. [5] have performed a study of the bulk electronic structure from a MOCVD grown sample on a sapphire (Al_2O_3) substrate. The sample was first etched in hydrochloric acid (HCl) ex situ and after insertion into the ultra-high vacuum (UHV) chamber annealed, no sputtering was employed.

Chao et al. [6] have reported on an ARUPS study mapping the surface electronic structure of a MOCVD grown sample on a silicon carbide (SiC) substrate. They have used sputtering with N ions and vacuum annealing as the cleaning method.

Dhesi et al. [7] have used the ARUPS technique to investigate the surface and bulk electronic structure of a MBE grown sample on Al_2O_3. They have cleaned the sample by first performing a Ga deposition followed by vacuum annealing, and then N ion sputtering followed by vacuum annealing. The work by Dhesi et al. has been compared with a one-step photoemission calculation of the GaN(000$\bar{1}$)-1 × 1-Ga surface made by Strasser et al. [8].

The surface electronic structure of p-type GaN has been studied by Ryan et al. [9]. They have studied a MBE grown sample on Al_2O_3, cleaned by N ion sputtering and vacuum annealing. GaN(0001)-1 × 1 or GaN(000$\bar{1}$)-1 × 1 are the only surface reconstruction that have been investigated by means of ARUPS so far.

This report consists of a detailed ARUPS study, from the carefully prepared stoichiometric GaN (0001)-1 × 1 surface of a Ga-polar sample grown by MOCVD. We are the first to report on an ARUPS study made on a stoichiometric GaN surface, achieved without employing any ion sputtering.

2. Experiment

ARUPS measurements were performed on the high-resolution spherical grating beamline (BL-33) at the MAX I synchrotron storage ring in Lund, Sweden [10,11]. The photoelectron energy analyser is a 75 mm radius hemispherical analyser (ARUPS-10, VG Microtech) with an electron entrance lens having an electronically variable acceptance angle, which in these measurements was set to ±2°. The total energy resolution of the analyser and monochromator was <100 meV. The base pressure in the system was $\sim 4 \times 10^{-11}$ mbar. The Fermi level position was determined from a clean Ta surface in good electrical contact with the sample. The incidence angle of the light (θ_i) for all spectra presented here was set to 45°. The emission angle (θ_e) of the detected electrons was varied by rotation of the analyser in the plane defined by the surface normal and the direction of the incident light. The synchrotron radiation is linearly polarised and the polarisation was in the plane of photoelectron detection.

ARUPS spectra were measured along the [10$\bar{1}$0] and [11$\bar{2}$0] azimuthal directions and in the [000$\bar{1}$] polar direction, which corresponds to the $\overline{\Gamma}$–$\overline{K}$–$\overline{M}$, $\overline{\Gamma}$–$\overline{M}$, and Γ–A directions in the 1 × 1 surface and bulk Brillouin zones (BZ), respectively, see Fig. 1.

The sample studied was a wurtzite structure GaN film, n-doped (Si) with a carrier concentration of $n = 4.65 \times 10^{17}$ cm^{-3} and a Hall electron mobility of $\mu_H = 376.5$ cm^2/V s. The doped GaN layer had a thickness of 0.72 μm, on top of an undoped GaN layer of 1.0 μm and a 20 nm buffer layer, grown on a sapphire (Al_2O_3) substrate by MOCVD. The sample surface normal was in the (0001) Ga-polar direction, as determined by an etching method [12,13]. The band gap for this sam-

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