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The electronic structure of the K/AlN nanointerface

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Abstract. The electronic structure of the AlN surface and the ultrathin K/AlN interface was studied using *in situ* photoelectron spectroscopy under ultra-high vacuum conditions. Core level spectra from the N 1*s*, Al 2*p* and K 3*p* and from the valence band were studied for the clean AlN surface and for the K/AlN interface in the regime of K submonolayer coatings. During K adsorption, significant changes in all the spectra were found. Surface states in the valence band region below the E_{VBM} were found. It was determined that the K/AlN interface has the semiconductor-like character.

Keywords: III-nitrides, aluminum nitride (AlN), interfaces, surface, photoelectron spectroscopy, electronic structure

Introduction

III-nitrides are widely used in modern micro- and optoelectronics. They are highly important for building heterostructures used in optical and high-power electronic devices (DenBaars et al. 2013). In the group of III-nitrides, AlN has a wide band gap of ~ 6.2 eV, low coefficient of thermal expansion, and high thermal conductivity. AlN is a favorable material for the development of UV light-emitting diodes and lasers (Taniyasu, Kasu 2008). Despite significant technical progress in the creation of high-quality materials, theoretical and experimental data on the electronic properties of AlN surface are scarce, including data on surface states, interface formation, band bending, etc. These properties are critical because they play a major role in nanostructures, where interfaces are of major importance. The electronic structure of the AlN surface has been studied in many aspects (Loughin et al. 1993; Magnuson et al. 2009; Strak et al. 2015), but information on the structure and electronic properties of metal/AlN interface is very limited (Kempisty et al. 2020; Kiranjot et al. 2020; Sznajder 2020). Recently, the electronic and photoemission properties of metal/$Al_xGa_{1-x}N$ interfaces, namely Cs/GaN, Ba/GaN, Ba/$Al_{0.16}Ga_{0.84}N$, Ba/$Al_{0.42}Ga_{0.58}N$, have been investigated (Benemanskaya et al. 2014; 2018a; 2018b; Timoshnev et al. 2020).

Photoelectron spectroscopy (PES) is one of the main techniques used to study the properties of atoms, molecules and solids, and the most important experimental technique to obtain the most complete information about the band structure of occupied electronic states because of its high sensitivity to chemical states. Recently, the surface and interface properties of group III nitrides have attracted close attention of researchers. Nitrides are widely used in the development and manufacture of optoelectronic devices in a wide spectral range from visible to UV light.

The aim of this work is to study the modification of the electronic structure of the K/AlN interface as a function of the K submonolayer coverage using photoelectron spectroscopy.

Materials and methods

Photoemission studies were carried out on an experimental RGL-station at the Russian-German beamline at BESSY II synchrotron radiation facility (Berlin, Germany) using the photon energies in the range from 100 eV to 650 eV. Studies were performed *in situ* in a high vacuum of 5×10^{10} Torr at room temperature. The photoelectrons emitted along the normal to the sample surface were recorded. The exciting beam fell on the sample surface at an angle of 45°. The normal photoemission spectra for the valence band area and from the N 1*s*, Al 2*p* and K 3*p* core levels were measured.

The AlN samples were grown on 6H-SiC/Si(111) substrates by chemical vapour deposition. The band-gap width corresponds to E_g = 6.2 eV. The samples of AlN were annealed *in situ* directly in a vacuum chamber at $T \sim 900$ K. Atomically clean potassium was adsorbed on the surface of the AlN sample from a standard calibrated source. Submonolayer coating from 0.1 monolayer (ML) to 0.9 ML of K was deposited on the clean AlN surface.

Results and discussion

Figure 1 shows normal photoemission spectra in the valence band area for the clean AlN surface (1) and for the K/AlN interface at the K monolayer coverage (2) – 0.9 ML. The excitation energy is $h\nu$ = 100 eV. The energy position of the E_{VBM} = 0 eV at the surface is determined by linear approximation of the low-energy shoulder of the spectrum of the valence band (VB). It is clear that, upon the adsorption of potassium, the intensity of photoemission from the valence band slightly decreases. In addition, a peak of the K 3*p* core level appears in the spectrum at binding energy of ~ 15.3 eV.

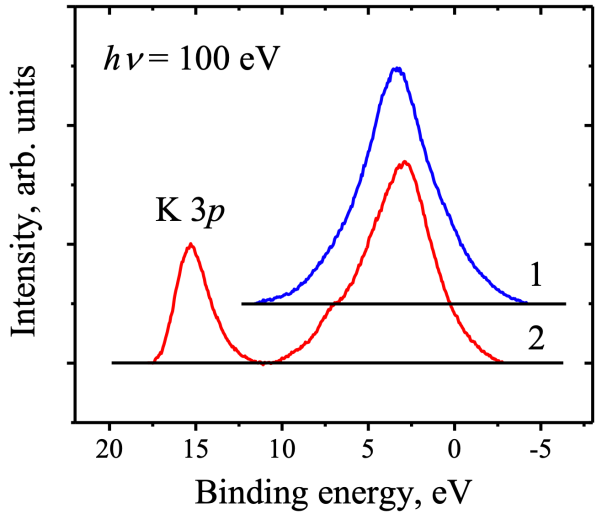

Fig.1. Normalized photoemission spectra from the VB for the clean AlN surface (1) and for the K/AlN interface (2) at the K coverage of 0.9 ML

For the clean AlN surface, the spectrum of the valence band area is described by the faintly structured bands S1 and S2 at the binding energies of – 0.1 eV and 5.9 eV relatively E_{VBM} with main VB maximum at ~ 2.9 eV (see fig. 2). The shape and the width of the spectrum of the valence band and surface states S1 and S2 spectra coincide well with the GaN and AlGaN photoemission results reported earlier (Benemanskaya et al. 2014; 2018a; 2018b; Timoshnev et al. 2020).

Figure 3 represents the photoemission spectra from the core level of N 1*s* for a clean AlN surface (fig. 3a) and a K/AlN interface (fig. 3b). The excitation energy is 470 eV. It is shown that the shape of the spectrum changes slightly upon adsorption of K. At the same time, the peak intensity decreases abruptly and its shift towards higher energies is observed. There is an intensity reduction of the N 1*s* peak by

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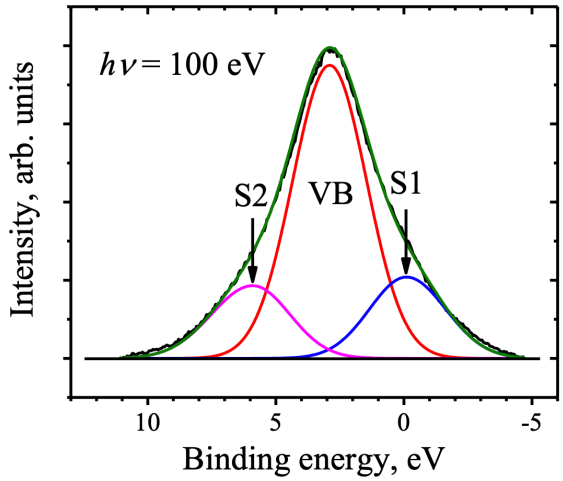

Fig. 2. Decomposition of the photoemission spectrum for the VB and surface states S1 and S2 for the clean AlN surface. The excitation energy is $h\nu$ = 100 eV

of ~ 2.1 times at the K coverage is 0.9 ML. The intensity of the peak of Al 2*p* decreased by ~ 1.4 times at 0.9 ML of K coverage (spectrum not shown). Since the photoemission intensity of the N 1*s* peak upon K adsorption decreased more than Al 2*p* peak it can be assumed that the AlN sample has a predominantly N-polar surface. The shift of the N 1*s* peak (~ 0.7 eV) towards higher binding energy was found, originating from the charge transfer with increasing the N-ionicity. Thus, changes in the Al 2*p* spectrum clearly show that K adsorbed atoms interact exclusively with the N atoms in the upper layer of the substrate AlN.

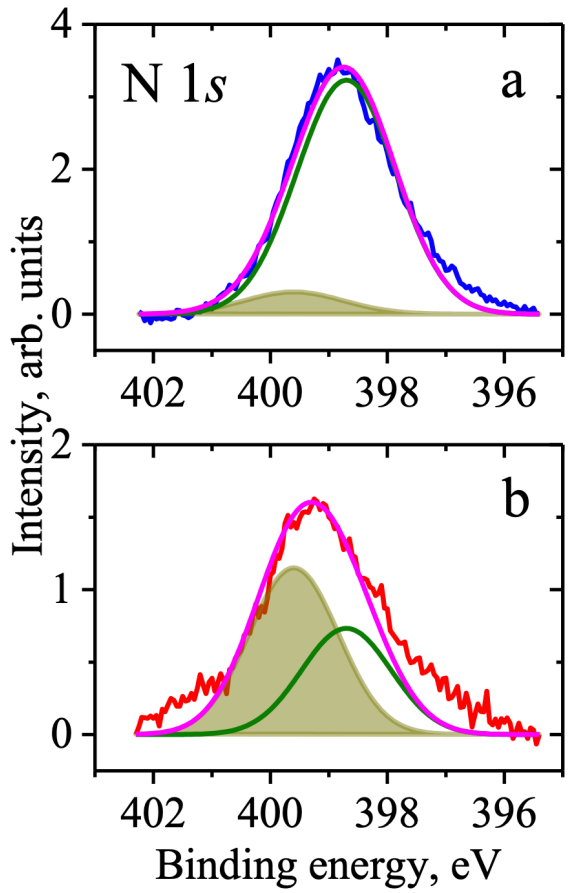

Fig. 3. Decomposition of the normalized photoemission spectra of the core level of N 1*s* for the clean AlN surface (a) and for K/AlN interface at K coating of 0.9 ML (b). Excitation energy $h\nu$ = 470 eV

Conclusions

The K adsorption on the AlN surface has been studied by synchrotron radiation photoelectron spectroscopy at different excitation energy in the range from 100 eV to 470 eV. The K deposition is found to modify the N 1*s* core level spectrum and the surface states spectra. For the pure AlN surface, the intrinsic surface states at the E_B of – 0.1 eV and 5.9 eV below E_{VBM} are found. The positive shift of the N 1*s* peak toward higher binding energy originates from charge transfer with increasing the N-ionicity.

Conflict of interest

The authors declare that there is no conflict of interest, either existing or potential.

Acknowledgements

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