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Initial interface study of Au deposition on GaN(0 0 0 1)

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Abstract

Synchrotron radiation photoelectron spectroscopy (SRPES) has been used to study the electronic structure of the Au/GaN(0 0 0 1) system at the initial growth stage. The peak fitting of Au4f$_{7/2}$ core-level and the energy shift of valence band indicate that Au–Ga alloy were formed in the interface reaction. According to the Ga3d signal intensity attenuation vs. the gold film thickness, the early growth mode is considered to be 3D mode above the reaction layer. By using the Linear Augmented Plane Wave method the density of states (DOS) for GaN and Au bulk are calculated within the framework of local functional theory. The theoretical results agree with the valence band structure quite well. The mechanism of interface reaction is discussed based on the experimental and theoretical results.

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Keywords: Growth mode; Au/GaN interface; SRPES; Valence band DOS; Alloy

1. Introduction

GaN is of significant importance for the fabrication of high-power and high-speed electronic devices [1–3]. Of late people have started paying much attention to this typical wide-band material and the focus mostly lies on the metal-GaN ohmic contact [4–9] because the performance of the GaN-based devices is greatly limited by the contact quality. It is well-known that gold is a potential candidate to produce high-quality ohmic contact for GaN because of its large work function. However, some basic characteristics of the Au/GaN interface are still ambiguous. For example, the growth mode of Au deposition on GaN surface has no clear answer, many literatures [10–12] give contradictory results. Furthermore, a careful examination of the interface valence band has not been reported and the mechanism of the interface reaction is also not very clear, especially in the initial growth stage.

In this paper, we have studied the growth mode of the Au deposition on the GaN surface and the interface electronic structure by synchrotron

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radiation photoelectron spectroscopy (SRPES). More attention is being paid on the Au4f band energy shift and the valence band evolution during the low-coverage metal deposition. The local partial density of states (PDOS) of the valence band is calculated within the framework of local functional theory and the mechanism of interface reaction is discussed based on the experimental and theoretical results.

2. Experiment

The experiment is performed at the surface physics station of NSRL (National Synchrotron Radiation Lab) at Hefei, China. This experiment station is mainly composed of a three-chamber VG multi-technique UHV system. It consists of a molecular beam epitaxy (MBE) chamber which has a thickness monitor TM400 from MAXTEK Inc, a pre-treatment chamber with a fast entry lock and an analysis chamber equipped with ARUPS10 hemispherical analyzer. Samples can be cleaned by cycles of Ar^+ ions etching and e-beam annealing in the pre-treatment chamber and transferred to the analysis chamber for SRPES. The XPS, LEED, RHEED and AES are also equipped and all these systems work under UHV conditions (better than 2×10^{-10} mbar). The beamline covers the energy range from 10 to 300 eV and the energy resolution ($E/\Delta E$) is better than 1000. More details of the experiment station and the related beamline are described elsewhere [13].

The sample used in the experiment is cut from GaN epitaxial film grown by MBE on sapphire substrate along the *c*-axis. An AlN layer of about 0.2 μm is grown as the buffer layer, followed by 0.7 μm of undoped GaN. The prepared sample is degreased in acetone and then rinsed in DI (de-ionized) water. After blow drying with N_2, the sample is loaded into the ultrahigh vacuum chamber. In order to remove carbon and oxygen contaminations on GaN surface, repetition of Ar-ion sputtering and annealing at 600 °C in the UHV is performed. With the above treatment, C 1s and O 1s peaks are not found in the XPS measurement and clear hexagonal lattice spots are observed on the RHEED pattern shown as Fig. 1(a). Then

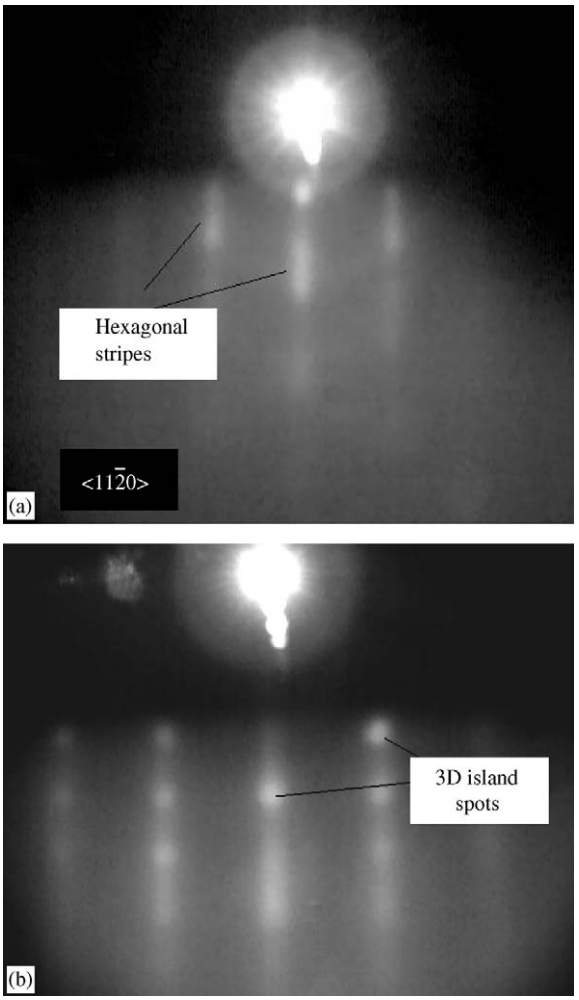

Fig. 1. RHEED patterns observed at the clean surface (a) and the surface covered by 12 Å gold film (b).

the high-purity Au (better than 99.99%) is evaporated in the K-cell at 1250 °C and the evaporation rate is about 1 Å/100 s measured by the quartz crystal thickness monitor. The temperature of the substrate is kept at 500 °C during the metal deposition. The SRPES scans of the Ga3d and Au4f core levels are recorded by 150 eV photon energy and the valence band is recorded by 24 eV photon energy after every deposition. The N1s core level is out of our synchrotron radiation energy range and investigated by XPS at the same time.