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XPS study of the formation of ultrathin GaN film on GaAs(1 0 0)

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Abstract

The nitridation of GaAs(1 0 0) surfaces has been studied using XPS spectroscopy, one of the best surface sensitive techniques. A glow discharge cell was used to produce a continuous plasma with a majority of N atomic species. We used the Ga3d and As3d core levels to monitor the chemical state of the surface and the coverage of the species. A theoretical model based on stacked layers allows to determine the optimal temperature of nitridation. Moreover, this model permits the determination of the thickness of the GaN layer. Varying time of nitridation from 10 min to 1 h, it is possible to obtain GaN layers with a thickness between 0.5 nm and 3 nm.

Keywords: XPS; Gallium arsenide; Gallium nitride; Semiconductor–semiconductor thin film structure; Heterojunctions

1. Introduction

Thin GaN films produced by nitridation, due to their high thermal and chemical stability, could be used for surface chemical passivation of GaAs [1]. Moreover, the high density of surface states of GaAs are known to induce surface Fermi level pinning [2]. GaN films are also expected to provide an effective electronic passivation because N atoms bonded with surface gallium [3] should not produce electronic states in the forbidden gap.

GaN materials are important for a variety of device applications: light emitters and detectors operating in the visible to UV spectral range [4], high power microwaves devices [5] or high frequency field effect transistors [6]. Hexagonal GaN films are usually grown on Al_2O_3 or SiC but GaAs(1 0 0) is a good candidate as substrate for the growth of cubic β-GaN. The best procedure to increase the quality of the c-GaN is achieved by a susbtrate nitridation before the deposition of a low temperature buffer layer [7]. In this case, the nitridation conditions are critical for this process.

In this paper we report the nitridation of GaAs(1 0 0) surface with a glow discharge cell. The composition of the nitridated layer was quantitatively studied using XPS spectroscopy.

Commercially available GaAs(1 0 0) wafers have been used in this work. Before introduction in the UHV chamber, samples were chemically cleaned using successive baths of deionised water, H_2SO_4 and hot methanol. The experiments were carried out in a home-built UHV chamber equipped with XPS system (dual anode Al–Mg X-ray source and hemispherical electron energy analyser). XPS experiments were performed using a Mg Kα source (1253.6 eV) at an incident angle of 50° (normal detection, pass energy of the analyser equal to 20 eV). After introduction in the UHV chamber, GaAs substrates were cleaned using 1 keV Ar^+ ions with a current density of 3 μA cm^{-2} at 6×10^{-5} Torr.

The nitridation process has been performed with a high voltage plasma discharge source (GDS). In this kind of nitrogen cell, continuous plasma was produced by a high voltage (about 2 kV) and a majority of N atomic species were created (nitrogen pressure: 1×10^{-4} Torr, ionic current: 1.0 μA cm^{-2}). Before nitridation the GaAs(1 0 0) substrates were heated to 400 °C during 1 h, then the samples were kept under a nitrogen flow for a chosen time.

2. In situ cleaning of the substrates

Ga3d and As3d peaks were recorded after ionic cleaning of GaAs. The background of spectra has been removed using the Shirley method. Cleaning and measurements have been made for eight substrates, and the results are reported in Fig. 1. One

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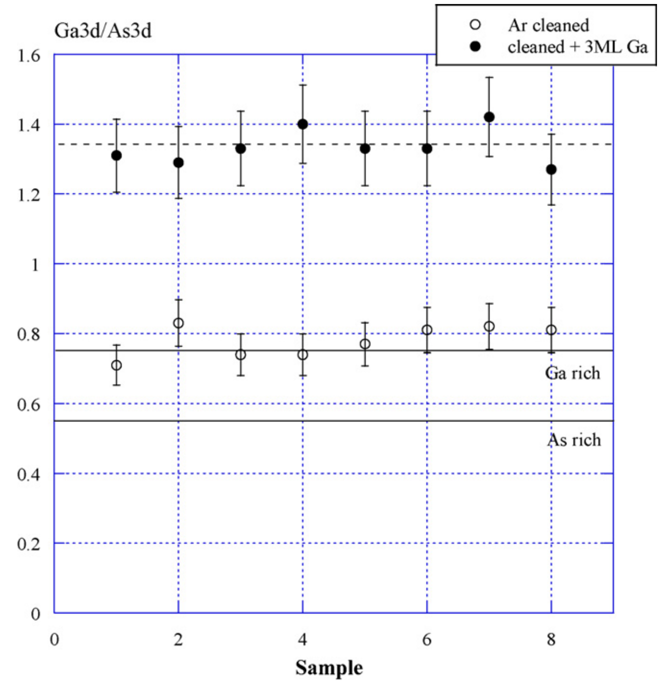

Fig. 1. Ga3d/As3d ratio after ionic cleaning (open circles) and after the deposition of 3 ML of metallic gallium (filled circles). The full and dashed lines correspond, respectively, to the theoretical ratios after cleaning and after gallium deposition.

can see that the ratio $R = I_{\mathrm{Ga3d}}/I_{\mathrm{As3d}}$ remains almost constant at a mean value of 0.77, this value can be compared with a theoretical calculation concerning the XPS signals of Ga3d and As3d.

A classical quantitative analysis of XPS can be resumed by a formula linking the flow Φ of photons, the number N of atoms in a layer at a depth z, the inelastic mean free path λ_i, the transmission of the electron analyser T at the kinetic energy of the XPS peak and the photoemission cross section σ of the element for a given transition. The assymetry factors were not be considered as we studied photoelectron peaks without decomposition. Finally, the contribution of an element x at a depth z in the total photoemission current will be:

$$dI_x = \sigma_x N_x T_x \Phi \exp\left(-\frac{z}{\lambda_{ix}}\right) \tag{1}$$

for a normal detection of photoelectrons.

This approach can be adapted to GaAs(1 0 0) substrates shematized by alternated layers of gallium and arsenic, we can introduce the distance d between two planes of Ga or As in GaAs. Then, considering the thickness z as a number of b layers, it will be equal to bd and N will be equal to Sdn where S is the studied surface and n, the density of atoms.

For a complete description of the substrate, we can introduce the attenuation factor $\alpha_{\mathrm{A}}^{\mathrm{B}}$ of an electron coming from an atom A in a B matrix:

$$\alpha_{\mathrm{A}}^{\mathrm{B}} = \exp\left(-\frac{d_{\mathrm{B}}}{\lambda_{i\mathrm{A}}}\right),$$

finally, the signal of photoelectrons coming from the atoms A at a depth z in a B matrix will be given by the formula:

$$I_{\mathrm{A}} = \sigma_{\mathrm{A}} T_{\mathrm{A}} \Phi S d_{\mathrm{B}} n_{\mathrm{A}} \exp\left(-\frac{bd_{\mathrm{B}}}{\lambda_{i\mathrm{A}}}\right) = S_{\mathrm{A}} \exp\left(-\frac{z}{\lambda_{i\mathrm{A}}}\right) \tag{2}$$

using S_{A} as a sensitivity factor of the element A.

The theoretical current of Ga3d photoelectrons is given by

$$I_{\mathrm{Ga3d}} = \frac{S_{\mathrm{Ga}}}{1-(\alpha_{\mathrm{Ga}}^{\mathrm{GaAs}})^2} \tag{3}$$

if the last layer of the substrate is Ga or:

$$I_{\mathrm{Ga3d}} = \frac{S_{\mathrm{Ga}}}{1-(\alpha_{\mathrm{Ga}}^{\mathrm{GaAs}})^2}\alpha_{\mathrm{Ga}}^{\mathrm{GaAs}} \tag{4}$$

if the last layer of the substrate is As.

The same calculations can be done for arsenic when replacing Ga by As in the two last equations. Then, we can consider the ratio $R = I_{\mathrm{Ga3d}}/I_{\mathrm{As3d}}$ which can get two values:

$$\text{for a rich Ga surface}: \quad R^{\mathrm{Ga}} = \frac{S_{\mathrm{Ga}}}{S_{\mathrm{As}}}\frac{1-(\alpha_{\mathrm{As}}^{\mathrm{GaAs}})^2}{1-(\alpha_{\mathrm{Ga}}^{\mathrm{GaAs}})^2}\frac{1}{\alpha_{\mathrm{As}}^{\mathrm{GaAs}}} \tag{5}$$

$$\text{for a rich As surface}: \quad R^{\mathrm{As}} = \frac{S_{\mathrm{Ga}}}{S_{\mathrm{As}}}\frac{1-(\alpha_{\mathrm{As}}^{\mathrm{GaAs}})^2}{1-(\alpha_{\mathrm{Ga}}^{\mathrm{GaAs}})^2}\alpha_{\mathrm{Ga}}^{\mathrm{GaAs}} \tag{6}$$

For a Ga-rich surface, a theoretical result of 0.76 is obtained whereas for a As-rich surface, $R_{\mathrm{net}}^{\mathrm{As}}$ is equal to 0.55.

Theoretical and experimental points have been reported in Fig. 1 for eight substrates. One can see easily that the surface can be considered as a rich Ga-surface in accordance with previous works of authors [8] and most of the literature results [9]. Nevertheless experimental points seems higher than the theoretical value, that shows a light gallium excess on the surface.

3. Nitridation of GaAs substrates

3.1. Determination of the nitridation temperature

The aim of this part was to determine the optimal temperature of nitridation to avoid arsenic migration and decomposition of the surface. In order to decrease the effect of surface cleaning, after ionic bombardment, a fixed quantity (3 ML) of metallic gallium was deposited on the cleaned surface of eight substrates. The quantity of gallium was monitored by a quartz balance. Each sample was heated at a different temperature. At each step the ratio $R = I_{\mathrm{Ga3d}}/I_{\mathrm{As3d}}$ was measured and reported in Figs. 1 and 2, respectively, for gallium deposition and heating.

Considering gallium deposition, one can see in Fig. 1 that the ratio R remains constant at a mean value of 1.33. This value is in accordance with the theoretical ratio calculated using the model of stacking layers: