# Nitridation of GaAs(001) Surface Studied by Auger Electron Spectroscopy

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## 1. Introduction

GaN compound, which is a proven perspective material for high power electronics and blue light emitting devices, is difficult to grow on the technologically well-established substrates, i.e. Si and GaAs, which is mostly due to the significant lattice mismatch of GaN with those materials. One of the methods of overcoming the above difficulty is to grow, prior to GaN growth, a thin "low-temperature" buffer layer on the top of GaAs, and the subsequent MBE growth on the top of that buffer layer has been shown to result in a good quality cubic phase GaN [1]. However, a deeper understanding of the mechanisms governing nitridation process, formation of the buffer layer and nitride growth is vital for further improvement of device performance. In the present study we used Auger electron spectroscopy (AES) and RHEED to investigate the processes taking place during interaction of active nitrogen species with the As-stabilized GaAs(001)- 2x4 surface.

### 2. Experiment

GaAs homoepitaxial layers with thickness of ~500 Å were deposited on the Si-doped GaAs (001) by MBE, the resultant surface exhibited (2x4) surface reconstruction. Nitridation was carried out in the Ga- and As- free atmosphere, and nitridation rate was controlled by a variable leak valve, through which a

flow of 1 ccm of N<sub>2</sub> gas was introduced into the RF plasma source. The process of nitridation was carried out for three substrate temperatures: room temperature (RT), 300°C and 500°C. To characterize the bonding and composition of the buffer layer growing during the nitridation process, the Auger signals of Ga-LMM (~1070 eV), As-LMM (~1230 eV) and N-KLL (~380 eV) transitions have been used. No traces of impurities, such as oxygen and carbon, have been detected on the original surface.

#### 3. Results and Discussion

Fig. 1 shows the dependencies of AES spectra of Ga, As and N on the nitrogen exposure duration for the substrate temperature of 300°C, as well as (for gallium and nitrogen) the spectra taken after subsequent thermal annealing at 620°C for 3 min together with those for a thick (d~1.5 $\mu$ m) MBEgrown GaN reference sample. It can be seen from this figure that all transitions exhibit a pronounced shift to lower kinetic energies (KE) as the nitridation proceeds, the said shift being especially apparent during the initial two minutes of nitridation. After 100 min of nitridation the apparent shift amounts to -1.5 eV for N- and As-originated signals, and -2.5 eV for Ga-originated one. It can also be seen that the spectral shape of the signals changes in the process of nitridation. Therefore, we could not use the peak-to-peak intensities to



Fig. 2 Spectral shapes of the N-, Ga- and As-originated AES signals during nitridation, as well as that after annealing at 620°C for 3 min (dashed curves). The topmost curves for N and Ga-signals are the spectra for the MBE-grown GaN reference sample.

characterize the compositional changes on the surface and in the subsurface region, but used, instead, the integrated intensities of the non-differentiated signals. The observed shifts in the spectra depend on the nitridation temperature, which is due to the temperature-dependent presence of various N- and As-related species, such as AsN, amorphous-As etc., on the surface during the nitridation process.

As it has been verified by XPS studies [2], nitridation of the GaAs (001) surface results in the formation of the disordered GaAsN compound as incoming N atoms substitute for As-atoms. The formation of the GaAsN phase leads to the observed low-KE shifts in the spectra, the last effect being caused by a gradual increase in the ionicity of the chemical bonding. Indeed, ionic character of the Ga-As and Ga-N bonds is 0.07 and 0.3, respectively. In the process of the GaAsN compound formation, as the ionicity of the bonding increases, the core energy levels of the constituting elements shift to higher binding energies [2]. Since the binding energy of the core levels increases, the KE of electrons emitted from those levels should decrease, which is in accordance with our experimental results.

It can be seen by examining Fig. 1 that, while Ga- and Nspectra exhibit the low-KE shift discussed earlier, the last spectra taken after the longest nitridation time of 100 min are not yet completely shifted to their spectral positions in the GaN sample. This is due to the fact that even after the longest nitridation time the subsurface GaAsN layer does not transform completely into GaN, which is evidenced by a large amount of As remaining in that region. However, thermal annealing of that GaAsN layer for several minutes at 620°C results in an almost complete transformation of this layer into GaN due to desorption of As from the subsurface region. The formation of GaN is evidenced by a drastic decrease (down to 0.03) in the relative As concentration on the surface, as well as by an examination of the spectral shapes shown in Fig. 1, showing the additional low-KE shift after thermal annealing for the N- and Ga-signals. It should be emphasized that the spectral shapes of both Ga- and Nsignals after annealing are almost identical to those of GaN reference.

The above is supported by our RHEED results showing that after only 1 min of nitridation the original (2x4)reconstruction of the initial GaAs surface is destroyed with an appearance of (1x1) pattern from unreconstructed surface. This (1x1) pattern remains discernible for about 5 min of nitridation, after which it disappears completely, giving rise to no pattern except for a smooth background. Thermal annealing, however, results in an appearance of the RHEED pattern characteristic of cubic GaN phase.

Fig. 2 shows the dependencies of apparent relative atomic concentrations of As and N on the nitrogen exposure duration for three nitridation temperatures. It can be seen that, as the nitridation proceeds, the concentration of nitrogen increases while that of arsenic decreases, which should be expected taking into account the substitutional (anion exchange) nature of the nitridation process. Ga concentration remains



Fig. 2 Dependencies of relative atomic concentrations of N and As in the subsurface region on the nitrogen exposure duration for three nitridation temperatures.

const during nitridation (not shown). Several other observations can be deduced from Fig. 2, i.e.

1) With the increase of the surface temperature the rate of rise of the N-concentration and that of decline of the Asconcentration increases at the initial stages of nitridation, and the point at which the concentration of N becomes equal to that of As shifts to shorter exposure times. Therefore, the nitridation rate increases with increase in the temperature; and 2) The nitridation process takes place mainly during the first 2-5 min of nitrogen exposure, after which the signals from all constituent elements level off. Therefore, only a few minutes of nitridation are sufficient for the buffer layer fabrication.

#### 4. Summary

A thin cubic-GaN buffer layer was prepared on the GaAs (001)-2x4 surface by nitridation of the surface, which takes place by substitution of As atoms by impinging N atoms with the formation of the disordered GaAsN phase, which crystallizes into cubic GaN after subsequent thermal annealing for several min at 620°C.

#### References

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