Transmission electron microscopy investigations of III-Nitride/Sapphire Interfaces at the atomic scale

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1. INTRODUCTION

The important characteristic of the wurzite structure of GaN grown along the [0001] direction is the polarity that essentially influences its physical properties. The most commonly used substrate for the growth of GaN is sapphire (Al_2O_3) which is nonpolar. Thus controlling the properties governing the selection of the polarity of the deposited films is one of the main problems in growth GaN on c-sapphire.

Despite of a number of theoretical and experimental studies [1], little is known on the atomic structure of the III-nitride/Al_2O_3 interfaces and the atomic processes that govern the polarity. This is mainly due to the fact that conventional transmission electron microscopes were not capable to resolve single oxygen and nitrogen atoms with high spatial resolution.

2. RESULTATS

2.1 Experimental conditions

The classical well-established GaN MOVPE growth process leads to Ga-polar films and consists of three essential steps:

I. Nitridation of sapphire surface in NH_3 flux at 1080 °C [2]

II. Deposition of a thin low temperature (580 – 650°C) nucleation GaN layer on top of the nitridated sapphire with subsequent annealing in NH_3 ambience by increasing the temperature up to 1000-1100°C [3]

III. High temperature epilayer growth. (1000-1100°C)

In the present work we study stages I and II by conventional (JEOL 2010F) and aberration corrected (FEI TITAN) transmission electron microscopes. HRTEM images with atomic resolution allowed us obtaining the polarity of nanometer thick layers and islands.

2.2 Study of nitridation process

Nitridation is an exposure of the sapphire surface to a NH_3 flux at a temperature around 1000°C. This nitridation leads to the formation of wurtzite film with an AlON composition by chemical transformation of the sapphire substrate[4]. In this work this step is studied in details, morphology, microstructure, strain state, chemical compositions and polarity of the nitridation layers are investigated using conventional (JEOL2010F) and aberration-corrected (TITAN) transmission electron microscopes (TEM) together with atomic force microscope (AFM). The cross-section analysis by TEM reveals the presence of Al-polar islands together with a continuous AlON layer (Fig. 1). The continuous AlON layer was observed to change from N-polar to Al-polar after 3-4 monolayers. The TEM images obtained in plan view (PV) enables us to characterize the dislocations in the structure after nitridation process.

2.3 Low temperature buffer layer study

Fig. 2 shows a cross-section image of GaN buffer layer grown on nitridated sapphire surface. The layer is formed of small columnar (40 nm) micrograins. These micrograins are misoriented both in plane and out of plane from each other and consist of mixture of cubic and hexagonal structures. The wurzite AlN layer under a buffer layer stays stable as observed by HAADF HRSTEM.

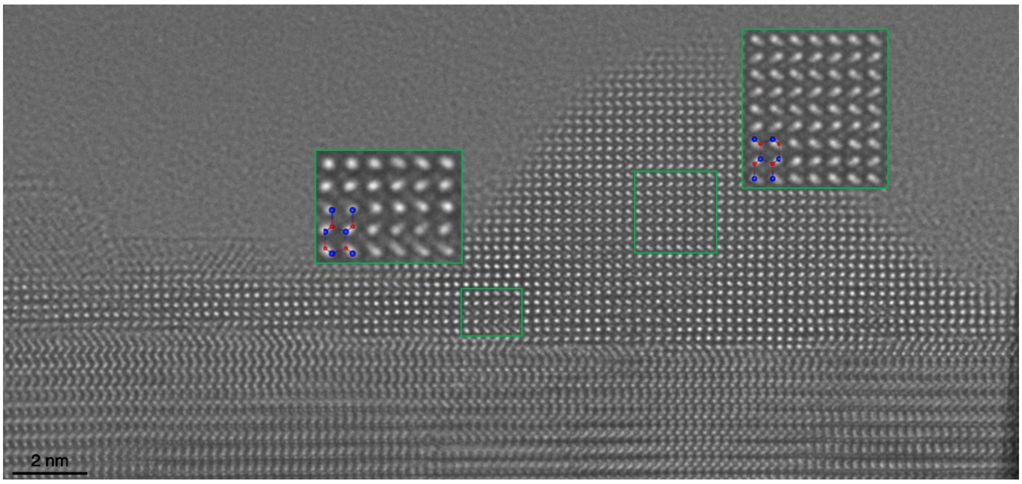

Fig. 1: CS HRTEM image of sapphire surface after 30 minutes annealing under NH_3 flux. The inserted squares show the different polarity of two regions: in the continuous layer near the base of the island and in the middle of the island. Blue circles indicate Al atoms and red circles – N-atoms.

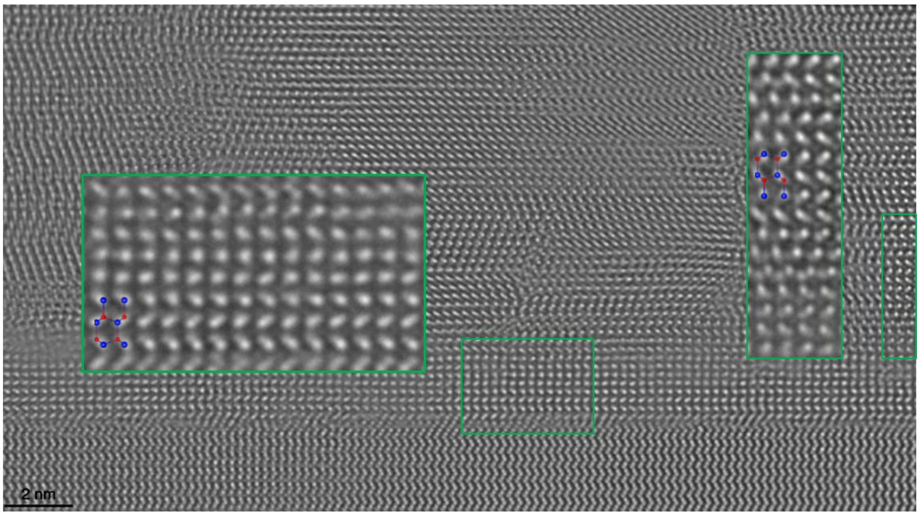

Fig.2: CS HRTEM image of GaN buffer layer grown on nitridated sapphire surface. The mixture of cubic and hexagonal structures can be observed. The inserted squares show the wurzite N-polar AlN layer and Ga-polar wurzite region of GaN buffer layer. Blue circles indicate Al (Ga) atoms and red circles – N-atoms.

3. CONCLUSION

The essential steps of classical GaN MOCVD growth process were studied in details by the use of conventional and abberation-corrected HRTEM. The polarity and the strain state of the layers were investigated. The switch from N-polar AlN to Al-polar AlN was observed after nitridation step. Subsequently grown GaN buffer layer is highly distorted and consists of misoriented columnar grains. The layer is a mixture of cubic and hexagonal material and shows Ga-polarity in its wurzite regions.

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