CAICISS Analysis for the Polarity Conversion of GaN Films grown on Nitrided Sapphire Substrates

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Recently, there were many papers reported on the determination of polarity of the GaN films and its correlation with the growth condition. However, the correlation between the polarity of GaN films and GaN buffer layer is still not very clear as well as the control method of the polarity of GaN films. In this work, we report our recent results on the control of the polarity of GaN films grown on nitrided sapphire substrates by low-pressure metalorganic vapor phase epitaxy (LP-MOVPE). The key step for the control of the polarity of GaN epilayers is to insert two monolayers of Al prior to the growth of GaN buffer layers, which will be hereafter referred as to TMA preflow.

The substrates were first thermally cleaned in H_2 ambient at 1100 ℃ for 10 min and then exposed to an ammonia gas flow of 1500 sccm for 90 sec at the same temperature. Prior to the deposition of GaN buffer layers and epilayers, the nitrided sapphires were exposed to a TMAl flow of 5 μmol/min at 550℃ for 2 to 30 sec. 20-nm-thick GaN buffer layers and 2.5-μm-thick GaN epilayers were then grown on nitrided sapphire substrates at 550 ℃ and 1080 ℃, respectively. In order to investigate the effects for the insertion of two monolayers of Al on the polarity conversion of GaN films, coaxial impact collision ion scattering spectroscopy (CAICISS, Shimadzu, TALIS-9700) was used. In this experiment, the dependence of Ga signal intensity on the incident angle of He^+ ion beam (2 keV) at the $[11\bar{2}0]$ azimuth of GaN films was studied for all samples.

Nitridation is one of the useful methods to improve the GaN quality. However, the surface of GaN epilayers exhibits usually hexagonal pyramidal morphology. It is well known that smooth epitaxial GaN films are usually Ga-face, which is defined as Ga polarity (+c), and films with hexagonal pyramidal morphology are N-face, which is defined as N polarity (-c).[2)] Because the nitrided sapphire substrates have N-terminated (0001) surface nature resulting in N-polarity of GaN films, it would be very difficult to grow the Ga-polarity GaN films with smooth surface. In order to grow the Ga-polar GaN films with smooth surface by changing the polarity of GaN films on nitrided sapphire substrates, we have grown GaN films with different TMAl preflow times. The surface of GaN film with 2 sec TMAl preflow showed still the hexagonal facets likewise the sample without TMAl preflow. However, the morphology of GaN films with TMAl preflow exceeding 5 sec was successfully changed into a flat

surface. These phenomena indicate that the TMAl preflow changed the polarity of GaN films.

The polarity of the GaN films with different TMAl preflow times was characterized by using CAICISS, and determined by comparison with the CACISS data already reported already for GaN[2] as well as ZnO.[3] Figure 1 shows the polarity variations of GaN films with different TMAl preflow times. Ga signal intensities were measured as a function of the incident angle of the He^+ ion beam at the $[11\bar{2}0]$ azimuth of GaN in CAICISS. As shown clearly in Figs. 1(a) and 1(c), the angular dependence of the Ga signal was quite different for GaN films deposited on nitrided sapphire without and with TMAl preflow of 5 sec. That is, GaN films grown on the nitrided sapphire without TMAl preflow have N polarity (-c), whereas GaN films grown using a TMAl preflow above 5 sec have Ga polarity (+c). However, the polarity of the sample with TMAl preflow of 2 sec is not fully changed into Ga-polar [Fig. 1(b)]. It is considered the sample with 2 sec TMAl preflow time was grown by mixed polar of N-polar and a few-percentages Ga-polar.

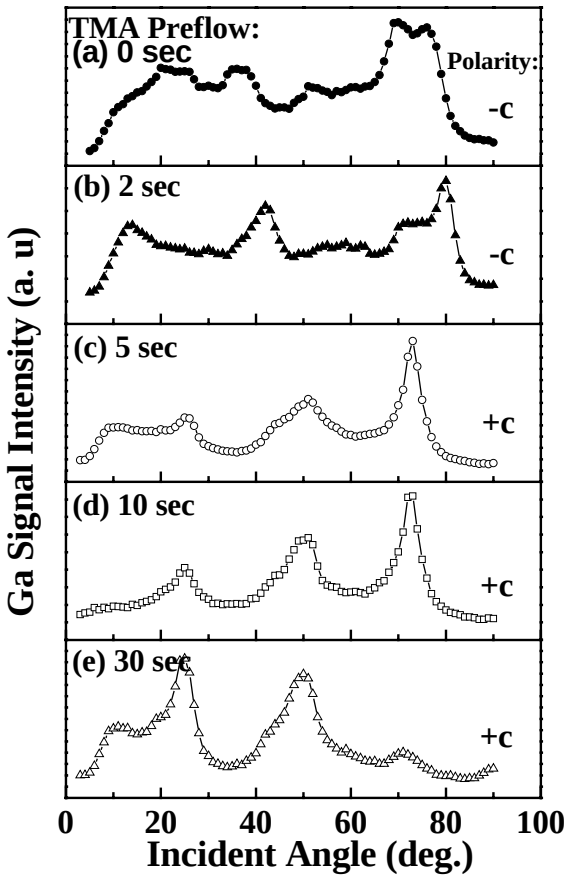

Fig. 1. The polarity variations of GaN films with TMAl preflow time.

Why the polarity of GaN could be changed? We propose a model to explain this. The model is represented as the structure containing two monolayers of Al. The staking sequence of the wurtzite GaN structure grown on nitrided sapphire substrates is like: …(AB)(AB)(AB)… When two monolayers of Al was inserted between GaN buffer layer and the nitrided sapphire substrates, the staking sequence of this structure will be changed into …(AB)(AB)(AB)**(A'A')**(BA)(BA)(BA)… So, GaN films with two monolayers of Al can be changed into Ga-polarity.

In conclusion, the GaN films grown without TMAl preflow showed N polarity, whereas those grown with TMAl preflow showed Ga polarity. So, we can conclude as follows; it is necessary to inserting a few monolayers of Al for the conversion of the polarity of GaN form N- to Ga-polar.

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