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Reducing dislocation density in GaN films using a cone-shaped patterned sapphire substrate

Hui-Youn Shin, S.K. Kwon *, Y.I. Chang, M.J. Cho, K.H. Park

Materials Characterization Group, LG Electronics Institute of Technology, 16 Woomyun-dong, Seocho-gu, Seoul 137-724, South Korea

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The threading dislocation (TD) density in GaN films grown directly on flat sapphire substrates is typically $>10^{10}/cm^2$, which can deteriorate the properties of GaN-based LEDs significantly. This paper reports an approach to reducing the TD density in a GaN layer using a variety of patterned sapphire substrates (PSS). A cone-shaped PSS produced by metal organic chemical vapor deposition (MOVCD) was used for GaN deposition. Three types of GaN specimens were prepared at the initial nucleation stage, middle growth stage and final growth stage. The TDs generated on the cone-shaped PSS were analyzed by transmission electron microscopy (TEM) and a strain mapping simulation using HRTEM images, which evaluated the residual strain distribution. A large number of TDs were generated and the residual strain by the lattice distortions remained above the top of the cone-shaped regions. However, no TDs and residual strain were observed at the slope of the cone-shaped regions. This might be due to the formation of a GaN layer by lateral overgrowth at the slope of the cone-shaped regions, resulting in less lattice mismatch and incoherency between the GaN and sapphire. In conclusion, the TD density in the GaN layer could be reduced significantly, approximately $10^7/cm^2$, using the cone-shaped PSS.

1. Introduction

Gallium nitride (GaN) is chemically and physically stable due to the strong bonding between atoms, and has a high thermal conductivity and electron saturation velocity. For these reasons, GaN is one of the most promising materials for applications as short-wavelength light emitters, such as light emitting diodes (LEDs) and laser diodes (LDs) in the green-to-ultraviolet range, and high-temperature electronic devices [1–3]. Generally, conventional GaN-based LEDs are grown on sapphire substrates. The crystal quality of the subsequent GaN epitaxial layer on the substrate can be improved by introducing a low-temperature GaN or an AlN nucleation layer. However, threading dislocations (TDs) with a density in the order of 10^9–$10^{12}/cm^2$, remain in the sample due to the large differences in lattice constants and thermal expansion coefficients between the GaN epitaxial layers and sapphire substrates [4], which may deteriorate the causal properties of GaN-based LEDs significantly. Therefore, the TDs density in the epitaxial layer needs to be reduced to improve the performance of nitride-based LEDs. Various techniques have been proposed to reduce the TD density [5].

Recently, it was reported that the TD density could be reduced successfully to the $10^6/cm^2$ range by epitaxial lateral overgrowth (ELOG) using stripe mask patterns on GaN [6,7]. Although this technique improved the crystallinity of the overgrown layer, it inherently suffered from inevitable growth interruption, in which a SiN_x or SiO_2 mask is deposited after the growth of a 1–2 μm-thick GaN layer. Additional mask-related drawbacks of this technique include possible impurity contamination and strain in the subsequently grown layers [8]. Therefore, in order to improve the performance of optoelectronic devices, a maskless, growth-interruption-free, angle-step overgrowth technique is desirable for reducing the TD density. This method has been reported previously, and a GaN layer with a low TD density was manufactured successfully using cantilever overgrowth on deeply trenched sapphire substrates [9]. In addition, the external efficiency in InGaN-based LEDs grown on patterned sapphire substrates (PSS) was enhanced without mask-related problems based on the effect of optical reflection from the side edge of the etched sapphire substrate [10]. However, although there has been considerable research on improving the optical properties and reducing the TD density with PSS applications, the cause and process of reducing the density of TDs on PSS is unclear.

With this background, the TD density in the GaN layer is of great importance, therefore we propose an approach to the mechanism for reducing the TD density in a GaN layer on a

* Corresponding author. Tel.: +82172091443; fax: +8225264928.
E-mail address: shk2th@hanafos.com (S.K. Kwon).

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cone-shaped PSS. This study was analyzed by transmission electron microscopy (TEM) combined with high-resolution TEM (HRTEM), and a strain mapping simulation to understand the TDs formation at the GaN/sapphire interface.

2. Experimental procedure

A PSS was manufactured using an inductively coupled plasma reactive ion etching (ICP-RIE) system. The width and height of the ridges were approximately 2.5 and 1.5 μm, respectively, and the interval of the ridges was approximately 1 μm. Therefore, the area of flat region was less than the cone-shaped region on approximately PSS. Furthermore, three types of GaN specimens were prepared at the initial nucleation stage, middle growth stage and final growth stage specimens. All layers of the specimen were grown on cone-shaped PSS using MOVCD. In this experiment, ammonia (NH_3) and trimethylgallium (TMGa) were used as the nitrogen and gallium sources, respectively, and pure H_2 was used as a carrier gas. The GaN growth rate of all specimens was 2 μm/h and the growth pressure of them was uniformly remained about 250 Torr. Initially, the specimen at the initial nucleation stage was composed of a low-temperature GaN (LT-GaN) layer, which was accomplished at 700 °C for 5 min with V/III flux ratio of 3000 as a buffer layer. The specimen at the middle growth stage, which was composed an undoped GaN (u-GaN) layer and a n-type doped GaN (n-GaN) layer on the LT-GaN/PSS, was produced at 1160 °C for 1 h with V/III flux ratio of 1500, followed by the addition of silicon (Si) as a doping element for n-GaN. Finally, the specimen in the final growth stage, which was composed of a u-GaN layer and n-GaN layer on the LT-GaN/PSS formed at 1160 °C for 2 h with V/III flux ratio of 1500.

The samples were examined by TEM, and associated techniques. The TEM specimens were prepared by mechanical polishing using a tripod polisher and ion milling. The prepared TEM specimens were examined using Philips CM 20 and FEI G2 microscopes operating at 200 kV. A strain mapping simulation was accomplished using Strain Determination Software v2.0, which is a geometrical phase method, designed and developed by Pedro L. Galindo [11]. This method involves filtering the image with an asymmetric filter at a Bragg spot of the Fourier transform of the HRTEM lattice image and performing an inverse Fourier transform. Therefore, the phase component of the resulting complex image provides useful information about the local displacement in a given direction to understand the formation of TDs at the GaN/sapphire interface.

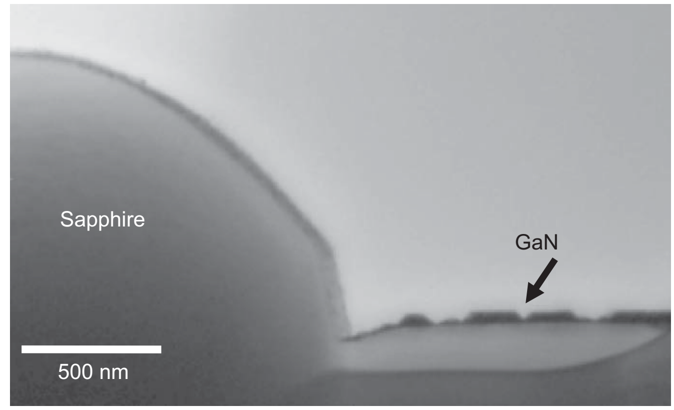

Fig. 1. Cross-sectional bright-field TEM image of the initial growth stage of a GaN layer grown on cone-shaped PSS. The direction vector of the electron beam is [2 $\bar{1}$ $\bar{1}$ 0]. The GaN nucleation was observed only on the flat sapphire region, but no nucleation was observed on the cone-shaped region.

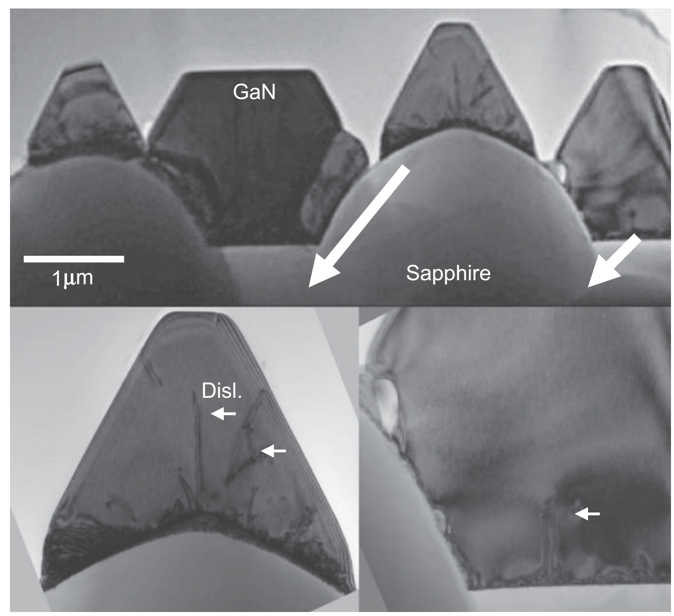

Fig. 2. Cross-sectional bright-field TEM images of the middle growth stage of GaN layer grown on cone-shaped PSS with the [2 $\bar{1}$ $\bar{1}$ 0] electron beam direction. The GaN crystallites had an island-shape, and a large number of TDs were generated above the top of the cone-shaped regions, which are accommodated the large lattice mismatch with the sapphire substrate.

3. Results and discussion

At the initial stage GaN nucleation on cone-shaped PSS was examined by preparing a specimen with only a LT-GaN layer deposited before high-temperature growth. The essential role of the LT-GaN as a buffer layer was both to supply a high density of nucleation centers with the same orientation as the substrate and promote lateral growth of the epitaxial film due to a decrease in interfacial free energy between the epitaxial film and substrate [12]. Therefore, the defect density decreases dramatically and high-quality GaN was formed above the high defect region. Fig. 1 shows a cross-sectional bright-field TEM image of the initial nucleation stage of a GaN layer grown on cone-shaped PSS. Considerable GaN nucleation with a 10 nm thickness was observed only on the flat sapphire region, but no nucleation was observed on the cone-shaped region. Therefore, the LT-GaN as a buffer layer was formed only on the flat sapphire region.

Fig. 2 shows cross-sectional bright-field TEM images of the middle growth stage of a GaN layer grown on cone-shaped PSS. According to this figure, GaN growth occurred on top of the cone-shaped region and on the flat sapphire region. The GaN crystallites had an island-shape, which were formed by lateral overgrowth to the slope of the cone-shaped regions. A large number of TDs were generated above the top of the cone-shaped regions, which are believed to accommodate the large lattice mismatch with the sapphire substrate (16%). On the other hand, a large number of TDs were generated above the flat sapphire regions, but there were less TDs propagated vertically to the GaN surface. The TDs propagation was reduced effectively because the area of flat regions on the PSS was conspicuously smaller than that of the cone-shaped regions, and the LT-GaN layer as a buffer was formed differently on the flat sapphire regions than on the cone-shaped regions.