Effects of AlGaN/AlN Stacked Interlayers on GaN Growth on Si (111)

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(Received 11 December 2009)

We report the growth of high quality and crack-free GaN film on Si (111) substrate using $Al_{0.2}Ga_{0.8}N$/AlN stacked interlayers. Compared with the previously used single AlN interlayer, the AlGaN/AlN stacked interlayers can more effectively reduce the tensile stress inside the GaN layer. The cross-sectional TEM image reveals the bending and annihilation of threading dislocations (TDs) in the overgrown GaN film which leads to a decrease of TD density.

PACS: 81. 15. Gh, 61. 72. Uj DOI: 10.1088/0256-307X/27/3/038103

Commercially available GaN based devices such as light emitting diodes are usually grown on sapphire or SiC by metalorganic chemical vapor deposition (MOCVD). However, in recent years, the advantages of silicon substrates, including low cost, availability of large and high-quality wafers, as well as superior thermal and electrical conductivity, make III-nitrides heteroepitaxy on Si attractive. However, the large lattice mismatch (17%) and the difference in thermal expansion coefficients (56%) between GaN and Si substrates lead to the formation of a great number of dislocations. The situation is worsened by the emergence of cracks in the films when the thickness of the deposited layer exceeds a critical value.

Up to date, various methods, such as inserting single or multi-AlN thin layers into GaN layer[1,2] or using AlN/GaN superlattice[3] and step-graded or composition-graded AlGaN/AlN stacked buffer layers between GaN and Si[4−8] have been developed to compensate for the large thermal tensile stress and prevent the formation of cracks. In these methods, the growth of AlN/GaN superlattices or step-graded AlGaN buffer layers needs a precise control of layer parameters and is strongly dependent on the experimental system. In comparison, inserting AlN interlayer into GaN is a simple and effective way to prevent the cracking of a GaN layer grown on Si. However, a tradeoff must be made between tensile stress reduction and threading dislocation (TD) induction in the top GaN layer using this technique. These effects are strongly dependent on the AlN growth temperature. Low-temperature AlN can be more effective in offering a compressive stress to compensate for the tensile stress during cooling. However, it tends to introduce more TDs into the top GaN layer.[9]

In this study, we grow a GaN film on a Si(111) substrate with an AlGaN intermediate layer between the AlN interlayer and the upper GaN layer. It is shown that, compared with a single AlN interlayer, this kind of AlGaN/AlN stacked interlayer structure can more effectively compensate for the tensile stress induced by thermal mismatch, as well as reduce the TD density. With the transmission electron microscopy (TEM) observation, we have confirmed an obvious reduction of TD density in the top GaN layer.

The samples used in this study were grown on Si(111) substrates in an Aixtron 2000HT MOCVD system. TMGa, TMAl, and ammonia were used as precursors for Ga, Al, and N, respectively. Prior to growth, the Si substrates were chemically cleaned to obtain a hydrogen-terminated surface. The growth started with Al pre-deposition on the Si substrate to avoid Si nitridation. After a 20-nm-thick AlN seed layer, a SiN_x layer was deposited to partially mask the AlN seed layer to achieve lateral overgrowth of GaN at its initial stage.[10,11] After the full coalescence of the first GaN layer, two different interlayer structures were grown, one was with a single AlN interlayer (sample A) and another consisted of an AlN interlayer and a 500-nm-thick $Al_{0.2}Ga_{0.8}N$ layer (sample B) which were used for comparison. Then, 1-μm-thick GaN was grown on top of the interlayer. The entire GaN epitaxial layer structure with AlGaN/AlN stacked interlayers is schematically shown in Fig. 1 and the total thickness of the epitaxial film was around 2.3 μm.

A cross-sectional TEM study was carried out on JEOL 2010F operated at 200 keV. TEM specimens were prepared using mechanical thinning followed by ion-milling. Micro-Raman spectroscopy in backscattering configuration was used to check the stress state of as-grown GaN layers by measuring the related phonon peak shift in the Raman spectra.

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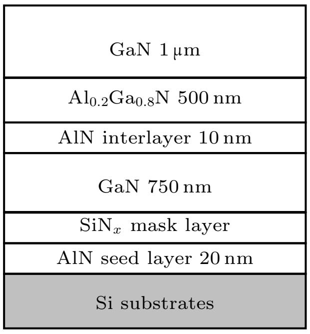

Fig. 1. Schematic diagram of epitaxial structure of GaN layers with AlGaN/AlN interlayers grown on Si (111) substrate.

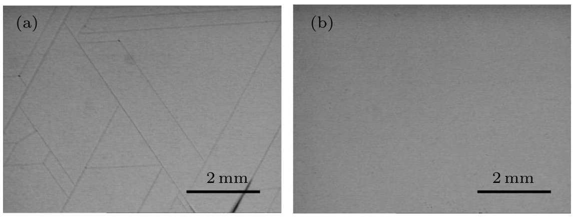

Fig. 2. Optical micrographs of the GaN surface grown on Si (111) substrate: (a) sample A, without AlGaN buffer layer and (b) sample B, with AlGaN buffer layer.

Figures 2(a) and 2(b) are optical micrographs which show the GaN surface morphology of samples A and B, respectively. In Fig. 2(a), although the AlN interlayer can partially compensate for the tensile stress in GaN during cooling, the GaN layer of sample A still suffers cracking. It is known that the AlN interlayer can impose a compressive stress to the GaN layer growing coherently on top of it because of the smaller in-plane lattice parameter of AlN. This compressive stress can thus partially offset the thermal tensile stress during temperature ramp-down. However, the GaN layer grown on the AlN interlayer tends to relax because of the 2.4% lattice mismatch between GaN and AlN. On the other hand, the additional introduction of an AlGaN buffer layer between GaN and AlN can result in a 'soft' transition in lattice constant. Therefore, the compressive lattice mismatch stress may be more effectively maintained to compensate for the tensile stress induced by thermal expansion mismatch. This way has really led to a smooth and crack-free GaN surface of the sample B, as shown in Fig. 2(b).

Raman scattering is performed on both the samples to quantitatively compare the stress state in GaN layers. Figure 3 shows the two typical Raman spectra for the GaN films of samples A and B, respectively (where the Raman spectrum is taken in an un-cracked region for sample A). In a backscattering geometry, both GaN E_2 (high) (E_2^h), and A_1(LO) phonon modes are observed. It is known that GaN E_2^h phonon peak is sensitive to the stress inside the layer.[12] For strain-free GaN the E_2^h peak is located at 567.5 cm^{-1} and this value has been taken as a standard one. Typically, the smaller the E_2^h phonon peak position shifts, the larger the residual tensile stress remains. The stress present in the GaN sample can be estimated by $\Delta\omega = 4.3\sigma_{xx}\,\mathrm{cm}^{-1}\mathrm{GPa}^{-1}$, where $\Delta\omega$ is the strain induced E_2^h peak shift and σ_{xx} is the in plane biaxial stress.[13,14] From Fig. 3, we can clearly see that the peak position of sample B ($565.9 \pm 0.2\,\mathrm{cm}^{-1}$) shifts to a frequency higher than that of sample A ($563.2 \pm 0.2\,\mathrm{cm}^{-1}$) and is closer to the value of strain-free GaN (567.5 cm^{-1}). The average tensile stress of sample A is estimated to be about 1.00 ± 0.05 GPa, and in sample B (with stacked AlGaN/AlN interlayer structure) the tensile stress is lower than in sample A, which is only about 0.37 ± 0.05 GPa. This result indicates that the AlGaN/AlN stacked interlayer structure can more effectively counteract the tensile stress of the GaN layer.

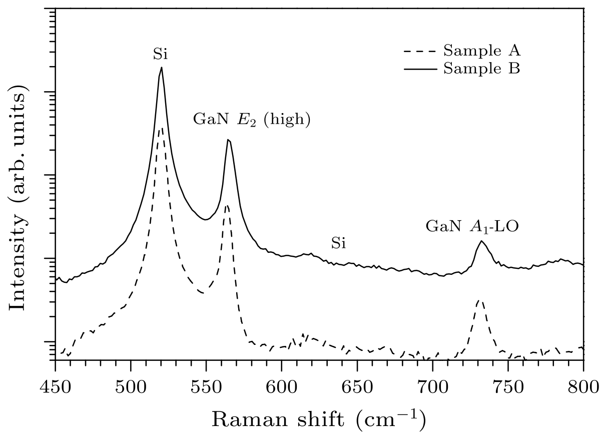

Fig. 3. Raman spectra of GaN layers in a backscattering geometry.

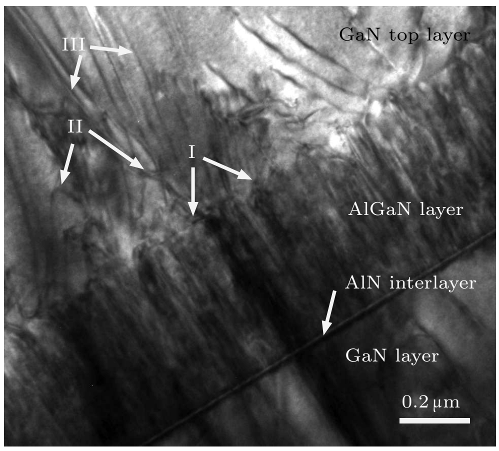

Fig. 4. Cross-sectional TEM image of GaN layers with AlGaN/AlN interlayers grown on the Si(111) substrate where the electron beam is along the $[1\bar{1}00]$ zone axis.

To study the structural evolution of GaN on the AlGaN buffer layer, cross-sectional TEM image of sample B was investigated. As shown in Fig. 4, the TEM images in this study are collected near the GaN

[1$\bar{1}$00] zone axis under multi-beam diffraction conditions so that all types of TDs can be revealed. It is found that a large density of TDs appears to originate from the AlGaN/AlN interface and thread through the whole AlGaN layer. This can be attributed to the mismatch between AlGaN and AlN layers and the three-dimensional (3D) growth mode of relaxed AlN layer on GaN.[9] It is interesting to note that many dislocation lines in the top GaN layer bend and deviate away from the growth direction. It can also be seen clearly that most TDs from AlGaN are terminated at or near the interface between GaN and AlGaN. It is worth pointing out that no additional TDs are generated at the AlGaN/GaN interface. Regarding TD's evolution in the top GaN layer, three general cases are observed, as indicated by white arrows: (i) Dislocations were trapped at or near the interface. (ii) TDs bend and react with nearby dislocations, forming dislocation half-loops in the region about 200 nm away from the interface. (iii) Dislocations keep threading through the layer to the surface. As can be seen from the TEM micrograph, cases (i) and (ii) are dominant ones, and thus lead to a significant drop in dislocation density on the GaN top layer.

Conventionally, about 90% of TDs present in the GaN layer grown on the Si(111) substrate are edge-type while about 10% are mixed ones. The amount of pure screw TDs is very small and can be neglected. It has been proposed that the bending of edge-type and mixed-type TDs occurs when the film is growing under a compressive stress.[15] Such bending results in a relaxation of compressive stress due to the formation of in-plane misfit segments.[16] In addition, the bending will enhance TD's interaction and annihilation, as shown in Fig. 4, leaving behind dislocation half-loops in GaN layer. As a result, the TD density in the top GaN layer decreases significantly. In fact, the bending of dislocation also symbolizes the intense compressive stress exerted by the AlN/AlGaN stack on the top GaN layer.

In summary, we have studied the effects of AlGaN/AlN stacked interlayers on properties of GaN grown on Si(111) by MOCVD. It is found that the AlGaN/AlN interlayers can more effectively compensate for the tensile stress inside GaN layer originating from thermal mismatch after cooling than a single AlN interlayer. In addition, a remarkable decrease of TD density in the GaN film overgrown on AlGaN is confirmed by cross-sectional TEM observations.

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