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A STUDY ON CRYSTALLINE MORPHOLOGY OF AN AlN THICK FILM GROWN ON THE TRENCH-PARTERNED α-Al_2O_3 USING X-RAY DIFRACTION

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Abstract: The crystalline morphology such as domain texturing, lattice tilting in a thick aluminum nitride (AlN) film grown on a trench-patterned α-Al_2O_3 template was investigated using X-ray diffraction measurements. The results clearly demonstrated that the trench-patterned template has a strong influence on the crystalline morphology in the thick AlN film. The crystalline morphology is anisotropic between the $[11\bar{2}0]$ and $[1\bar{1}00]$ directions. The AlN film contains several crystal domains, arranged along the $[11\bar{2}0]$ direction and tilted toward each other in this direction but parallel to each other in the $[1\bar{1}00]$ direction. These results can be attributed to the influence of the growth mechanism of the AlN film on the trench-patterned α-Al_2O_3 template and the elastic relaxation of strain along the growth direction.

Key words: AlN film; crystal domain; X-ray diffraction; trench-patterned template; crystal growth.

1. Introduction

Aluminum nitride (AlN) has attracted a significant amount of research interest in undeveloped fields such as deep ultraviolet light emitting diodes, lasers and high frequency electronic devices because of its wide bandgap energy of 6.2 eV [1-3]. Because of a lack of a large area bulk AlN substrate, epitaxial growth of AlN films on α-Al_2O_3 substrates are promising substitutes. α-Al_2O_3 substrates have been used for growing AlN films because: (1) α-Al_2O_3 and AlN have similar crystal structures, (2) their lattice and thermal mismatches are small, and (3) α-Al_2O_3 is cheap. Additionally, the use of trench-patterned templates fabricated on α-Al_2O_3 substrates has been shown to improve the crystalline quality of AlN films remarkably such as dislocation density reduction and crack suppression [4,5]. As has already been clarified in the previous report [5], the growth of the AlN films on trench-patterned templates includes the epitaxial lateral overgrowth (ELO) at the terrace, nucleation at the trench, and merging of the grown crystals. Because of this complicated crystal growth mechanism, there might be some crystalline morphology variations such as domain texturing and lattice tilting fluctuation in the films, which is still unclear at present.

The elucidation of the crystalline morphology of AlN films will allow us to not only understand the detailed mechanisms of crystal growth, but also propose practical process schemes for growing high quality crystalline AlN films. In this article, we investigate the crystalline morphology of a thick AlN film epitaxially grown on a trench-patterned α-Al_2O_3 template using X-ray diffraction.

2. Experimental details

The sample fabrication process is shown in Fig. 1. Firstly, as shown in Fig. 1(a), a trench pattern was formed in the $[1\bar{1}00]$ direction and periodically arranged in the $[11\bar{2}0]$ direction on a α-Al_2O_3 substrate using a reactive ion etching (RIE) technique. The orientation of the α-Al_2O_3 substrate is [0001]. Trench depth was set at 1.5 µm, while terrace and trench widths were both set at 2.0 µm. The trench-patterned α-Al_2O_3 template was then used as a substrate for AlN film growth. Finally, as shown in Fig. 1(b), a 8.6-µm-thick AlN film was grown using a low-pressure hydride vapor phase epitaxy

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(HVPE) system with infrared lamps as heaters. The growth pressure was 30 Torr and the growth temperature range was about 1400-1500°C. NH_3, Al, and HCl were used as source materials. N_2 and H_2 were used as carrier gases. Figure 1(c) shows a cross-sectional scanning electron microscopy (SEM) image of the thick AlN film grown on the trench-patterned α-Al_2O_3 template. Here, it can be observed that the voids form tunnels running along the $[1\bar{1}00]$ direction over the trenches and are arranged periodically in the $[11\bar{2}0]$ direction at 4-µm intervals. In addition, because the cross-section of the AlN film is not smooth and flat, the SEM image shows the nonuniform colour in the whole AlN film.

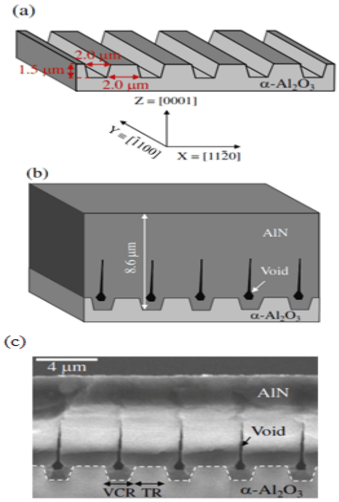

Fig. 1. *Schematic diagrams of the sample fabrication process: (a) a trench-patterned α-Al_2O_3 template; (b) a thick AlN film grown on the trench-patterned α-Al_2O_3 template. (c) Cross-sectional SEM image of the sample. The white dashed line indicates the interface between the grown AlN film and α-Al_2O_3 template. VCR and TR indicate void-containing trench and terrace regions*

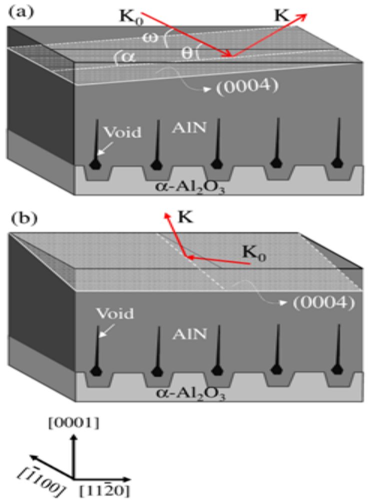

Fig. 2. *Diffraction geometries of XRD for AlN (0004) Bragg reflections along the directions of (a) $[11\bar{2}0]$ and (b) $[1\bar{1}00]$. **K_0** and **K** are incident and diffracted X-ray beams, respectively. ω, θ, and α indicate an incident angle of the X-ray beam with respect to the film surface, the Bragg angle and the tilt angle of (0004) planes with respect to the film surface, respectively*

In order to clarify the crystalline morphology of the thick AlN film such as domain texturing and lattice tilting, 2θ-ω X-ray difraction (XRD) measurements were performed using the Bruker D8 Discover system and the symmetric AlN (0004) Bragg reflection. XRD measurements were performed with two kinds of X-ray beam incidences which were perpendicular and parallel to the trench direction. Figures 2(a) and (b) show schematic diagrams of AlN (0004) XRD measurements in the $[11\bar{2}0]$ and $[1\bar{1}00]$ directions, respectively. The wavelength and the probe size of the X-ray beam were 0.15418 nm, and 100 µm × 100 µm, respectively.

3. Results and discussion

Figure 3 shows the results of 2θ-α XRD measurements from AlN (0004) lattice planes. Here, the tilt angle α of (0004) planes with respect to the film surface is determined by the difference between Bragg angle θ and the incident angle ω of the X-ray beam with respect to the film surface. It can be seen in Fig. 3(a) that the 2θ-α map of XRD in the $[11\bar{2}0]$ direction comprises multiple diffraction peaks with differences seen in tilt angles and peak intensities. This indicates that the AlN film contains several crystal domains, arranged along the $[11\bar{2}0]$ direction and tilted toward each other in this direction. Howerver, these multiple diffraction peaks have almost the same value of 2θ. This reflects that the difference in crystal constants of the crystal domains in the AlN film is negligible. In contrast, the 2θ-α map of XRD in the $[1\bar{1}00]$ direction comprises a single peak, as shown in Fig. 3(b). This indicates that the crystal domains in the AlN film are parallel to each other in this direction. These results demonstrate an anisotropic crystalline morphology of epitaxial thick AlN films grown on trench-patterned α-Al_2O_3 templates due to the anisotropy in structure of trench- patterned templates.

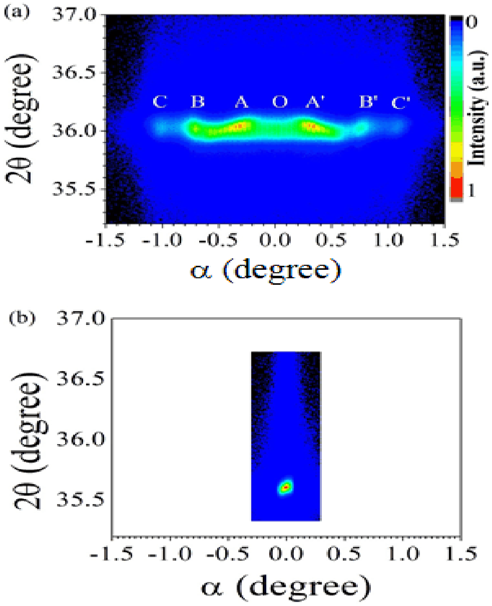

Fig. 3. *2θ-α maps obtained from XRD measurements on AlN (0004) lattice planes in the directions of (a) $[11\bar{2}0]$ and (b) $[1\bar{1}00]$. Symbols A, B, C, O, A', B', and C' indicate main diffraction peaks*

The above results can be attributed to the influence of the complicated growth mechanism of the AlN film on the trench-patterned α-Al_2O_3 template during HVPE and elastic relaxation of strain along the growth direction. As has already been clarified in the previous report [5], there are four different types of AlN growth at different locations on the trench-patterned α-Al_2O_3 template shown in Fig. 4: (I) vertical growth from the α-Al_2O_3 surface in the trenches, (II) lateral growth from the sidewalls of the α-Al_2O_3 terraces, (III) vertical growth from the top of the α-Al_2O_3 terraces, and (IV) lateral growth from Region III over the trenches. Figure 5 illustrates a simple model showing the tilting of AlN $(11\bar{2}0)$ lattice planes in Region IV near sidewalls of Region III. Because of elastic relaxation of the compressive strain component in the $[11\bar{2}0]$ direction along the [0001] growth direction [6], AlN $(11\bar{2}0)$ lattice planes in Region IV near sidewalls of Region III are tilted toward the $[11\bar{2}0]$ direction [7]. As a result, AlN crystal domains in Region IV are tilted toward this direction as indicated by the white arrows in Fig. 4. In contrast, the AlN film grows uniformly in the $[1\bar{1}00]$ direction on the trench and terrace, reflecting that crystal domains in the AlN film are parallel to each other in this direction.

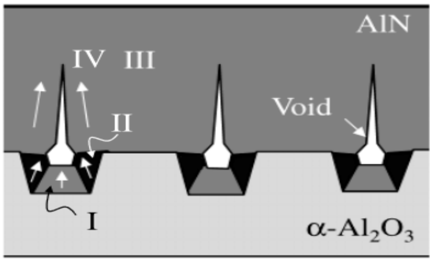

Fig. 4. *The growth mechanism model for a thick AlN film on a trench-patterned α-Al_2O_3 template. The white arrows indicate the c-axis orientation of crystal domains with respect to the surface normal in different growth regions*

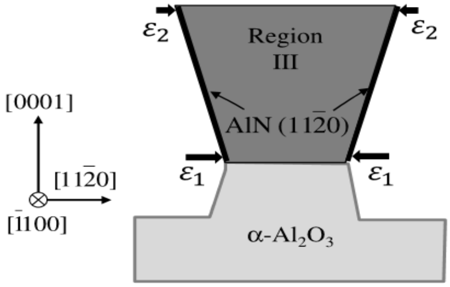

Fig 5. *A simple model showing the tilting of AlN $(11\bar{2}0)$ lattice planes in Region IV near sidewalls of Region III. ε_1 and ε_2 indicate compressive strains along the $[11\bar{2}0]$ direction near the AlN/α-Al_2O_3 interface and AlN surface, respectively*

4. Conclusion

We investigated the crystalline morphology of the thick AlN film epitaxially grown on the trench-patterned α-Al_2O_3 template by using XRD measurements. The results clearly demonstrated that the crystalline morphology of the thick AlN film is strongly influenced by the trench-patterned template. The crystalline morphology is anisotropic between the $[11\bar{2}0]$ and $[1\bar{1}00]$ directions. The AlN film contains several crystal domains, arranged along the $[11\bar{2}0]$ direction and tilted toward each other in this direction but parallel to each other in the $[1\bar{1}00]$ direction. The results can be attributed to the influence of the growth mechanism of the AlN film on the trench-patterned α-Al_2O_3 template during HVPE and elastic relaxation of strain along the growth direction. The anisotropy in the crystalline morphology of the AlN film corresponds to that of the trench patterned α-Al_2O_3 template. Therefore, in order to reduce this anisotropy, symmetric trench-patterned α-Al_2O_3 templates can be expected to facilitate crystal growth. In addition, an AlN buffer layer may be grown on the α-Al_2O_3 substrate in order to reduce the large lattice tilting fluctuation in the AlN film.

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NGHIÊN CỨU HÌNH THÁI HỌC TINH THỂ CỦA MÀNG DÀY AlN CHẾ TẠO TRÊN ĐẾ ĐƯỢC TẠO RÃNH α-Al_2O_3 BẰNG NHIỄU XẠ TIA X

Tóm tắt: Hình thái học tinh thể như cấu trúc miền, sự nghiêng mạng trong màng tinh thể nhôm nitrua (AlN) đã được nghiên cứu sử dụng các phép đo nhiễu xạ tia X. Các kết quả cho thấy đế tạo rãnh α-Al_2O_3 có ảnh hưởng mạnh đến hình thái học tinh thể của màng AlN. Hình thái học tinh thể của màng AlN có tính chất bất đẳng hướng giữa hai hướng tinh thể $[11\bar{2}0]$ và $[1\bar{1}00]$. Màng tinh thể AlN bao gồm một vài miền sắp xếp theo hướng $[11\bar{2}0]$ và nghiêng theo các góc khác nhau đối với hướng này. Tuy nhiên, các miền tinh thể của màng AlN lại định hướng song song nhau trong hướng $[1\bar{1}00]$. Các kết quả này là do ảnh hưởng của cơ chế phát triển của màng AlN trên đế tạo rãnh α-Al_2O_3 và sự giãn đàn hồi của biến dạng dọc theo hướng phát triển của màng.

Từ khóa: màng AlN; miền tinh thể; nhiễu xạ tia X; đế được tạo rãnh; chế tạo tinh thể.