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4H-polytype AlN grown on 4H-SiC$(11\bar{2}0)$ substrate by polytype replication

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4H-polytype AlN has been grown on a 4H-SiC substrate with the $(11\bar{2}0)$ face via plasma-assisted molecular-beam epitaxy. The microscopic structure of the AlN/4H-SiC interface was examined using high-resolution transmission electron microscopy, and the polytype replication of the 4H structure from the 4H-SiC$(11\bar{2}0)$ substrate was evidently confirmed. The x-ray rocking curve of $(11\bar{2}0)$ diffraction for the single crystalline 4H-AlN epilayer exhibited a very small linewidth of 90 arc sec, suggesting noticeably small tilting around the $[11\bar{2}0]$ direction. The excellent crystalline quality is probably owing to the polytype matching between the 4H-AlN epilayer and the 4H-SiC substrate, which resulted in remarkable reduction of defects at the interface. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1636533]

III-nitride compounds with a nonpolar face have attracted more and more interest to provide a promising means of eliminating polarization-induced electric fields in nitride-related devices utilizing heterostructure.[1] There have been some reports concerning growth of nitrides with a nonpolar face, but the crystalline quality is still inferior to that of technologically matured polar (0001) epilayer.[2,3] A nonpolar face of hexagonal SiC is suitable owing to its small lattice mismatch with AlN (~1%). We have reported the growth of AlN on 6H-SiC$(11\bar{2}0)$ substrates via plasma-assisted molecular-beam epitaxy (PA–MBE).[4] The SiC$(11\bar{2}0)$ surface has a unique atomic arrangement containing the stacking structure along the c axis. If an AlN epilayer inherits the arrangement, the polytype of SiC substrate will be replicated to the epilayer (atomic template effect). From the results of reflection high-energy electron diffraction (RHEED) and Raman scattering spectroscopy, the epitaxial relationship was revealed to be $a_{\mathrm{AlN}} \| a_{\mathrm{SiC}}$ and $c_{\mathrm{AlN}} \| c_{\mathrm{SiC}}$. However, the polytype of the AlN epilayer was a 2H structure, the stable structure of AlN, i.e., the atomic template effect of the substrate did not work well. The x-ray diffraction (XRD) measurement indicated the poor crystalline quality, which was attributed to many defects originated from the polytype mismatch between the AlN epilayer (2H:ABABAB···) and the SiC substrate (6H:ABCACB···).

In this study, the growth of AlN on a 4H-SiC$(11\bar{2}0)$ substrate, which has a different stacking structure (4H:ABCB···) compared to 6H-SiC, was studied, and the influence of SiC substrate polytype on the crystalline structure of the AlN epilayer was investigated by means of RHEED, high-resolution transmission electron microscopy (HRTEM), and XRD. We found that the atomic template effect does work in the AlN/4H-SiC$(11\bar{2}0)$ system, i.e., high-quality 4H-AlN can be grown on 4H-SiC$(11\bar{2}0)$.

The substrates used in this study were commercially available 4H- and 6H-SiC wafers with the $(11\bar{2}0)$ face. The substrates with a size of 7×8 mm^2 were first degreased using conventional organic solvents and dipped in HCl, HCl $+\mathrm{HNO_3}$ (3:1), and HF solutions, and then loaded into a MBE chamber. 380-nm-thick AlN epilayers were grown by PA–MBE using an effusion cell for Al evaporation and an EPI Unibulb rf plasma cell for producing active nitrogen. The substrate temperature was measured using a thermocouple located just behind the substrate. Prior to AlN growth, the substrates were thermally cleaned at 1000 °C for 30 min. AlN growth was carried out at 1000 °C under the following condition: an Al beam equivalent pressure of 4.7×10^{-7} Torr, a nitrogen flow rate of 0.5 sccm, and a rf power of 400 W. The growth rate under this condition was 380 nm/h.

In situ RHEED monitoring was conducted during AlN growth to investigate the polytype of AlN epilayer. Figure 1(a) shows the RHEED pattern of AlN epilayer grown on a 4H-SiC$(11\bar{2}0)$ substrate along the [0001] azimuth. In view of RHEED indices, the pattern agrees with that of the 4H structure, whose theoretical diffraction spots are presented in

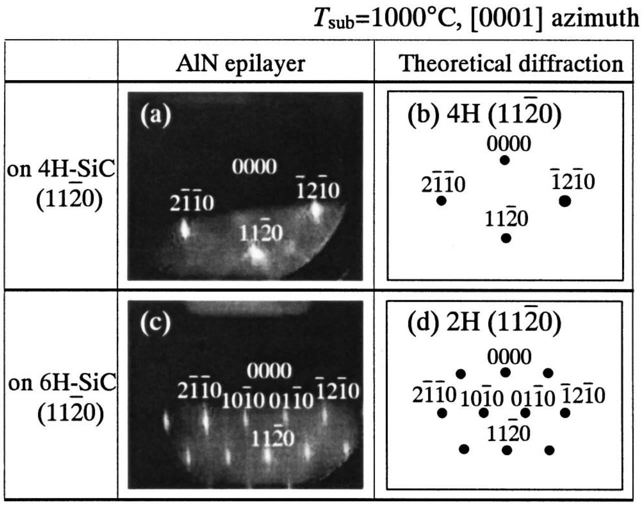

FIG. 1. RHEED patterns during AlN growth on a 4H-SiC$(11\bar{2}0)$ substrate (a) and on a 6H-SiC$(11\bar{2}0)$ substrate (c). (b) and (d) are theoretical diffraction spots from $(11\bar{2}0)$ surface for 4H and 2H structures along [0001] azimuth.

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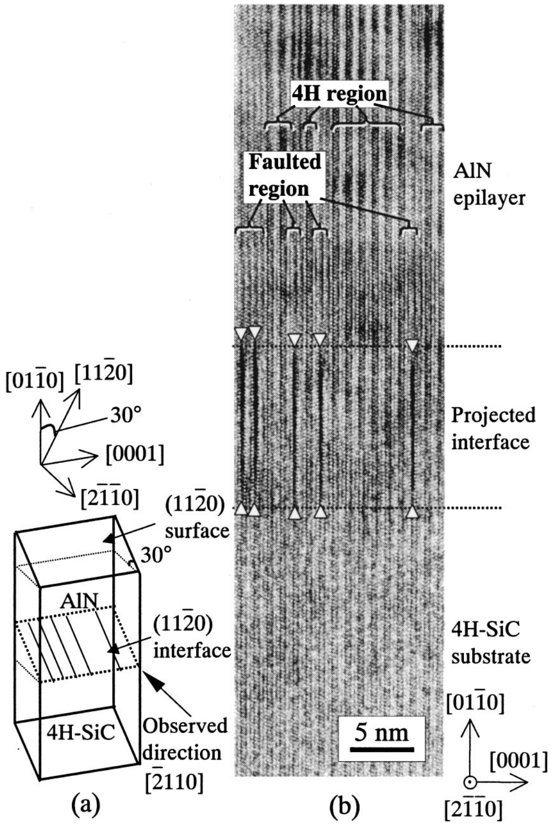

FIG. 2. Schematic of fabricated specimen (a) and lattice image of the AlN/4H-SiC$(11\bar{2}0)$ interface region (b).

Fig. 1(b). This RHEED evolution clearly indicates that the polytype of the 4H-SiC$(11\bar{2}0)$ substrate was replicated to the AlN epilayer. This is a completely different result from that of 2H-AlN growth on a 6H-SiC$(11\bar{2}0)$ substrate,^{4} as shown in Figs. 1(c) and 1(d).

The microscopic structure of the AlN/4H-SiC$(11\bar{2}0)$ interface was investigated by using HRTEM. The microscopy was performed on a Hitachi H-9000NAR microscope operating at 300 kV. In order to clarify the polytype of AlN epilayer from the stacking sequence, the incident electron beam along the $\langle 11\bar{2}0 \rangle$ zone axis should be employed. To achieve the geometry, a cross-sectional TEM specimen was cut from the wafer with a 30° inclination as shown in Fig. 2(a). The specimen was prepared by mechanical thinning and Ar ion milling. Figure 2(b) shows the lattice image of the AlN/4H-SiC heterostructure. As seen in the 4H-SiC substrate region, one set of dark and bright bands corresponds to one unit cell of the 4H structure (1.0 nm). The AlN epilayer has just the same dark and bright bands, indicating successful polytype replication from the 4H-SiC substrate, i.e., growth of 4H-AlN. Some regions do not have the 4H structure, i.e., faulted. Dark lines were observed at the interface region [see indications in Fig. 2(b)]. Since the length of dark lines agree with $\tan 30° \times$specimen thickness (20 nm), and the beginning and end are well aligned, the dark lines probably correspond to threading line defects along the $[1\bar{1}00]$ direction (parallel to the interface). The schematic diagram shown in Fig. 3 represents a possible structure of faulted region. The faulted regions were located just above the line defects. In other words, the atomic arrangement of the 4H structure was not replicated from the 4H-SiC substrate across the line defects. These line defects were probably generated at the initial stage of AlN growth. Therefore, the optimization of the initial growth condition will reduce the defects as well as the faulted regions in 4H-AlN.

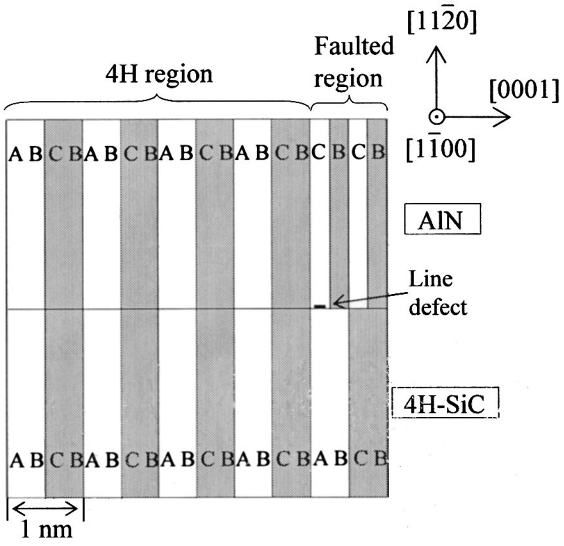

FIG. 3. Schematic diagram of a 4H-AlN/4H-SiC$(11\bar{2}0)$ heterostructure and the possible structure of the faulted region.

The x-ray rocking curves (XRC) of $(11\bar{2}0)$ diffraction for 380-nm-thick AlN epilayers grown on 4H- and 6H-SiC$(11\bar{2}0)$ substrates were measured to examine the crystalline quality. Two different x-ray incident geometries parallel and perpendicular to the $[1\bar{1}00]$ direction were examined. Figures 4(a) and 4(b) show the XRC profiles for the AlN epilayer grown on the 4H-SiC$(11\bar{2}0)$ substrate in those two geometries. There was no large difference in $(11\bar{2}0)$ diffraction between those two geometries. The full width at half maximum (FWHM) exhibited a very small value of 90

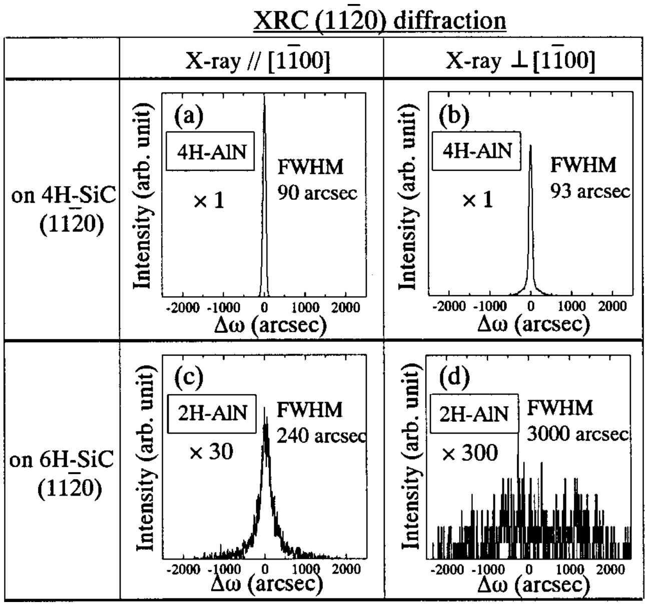

FIG. 4. XRC profiles on $(11\bar{2}0)$ diffraction for 380-nm-thick AlN epilayers on the 4H-SiC$(11\bar{2}0)$ substrate [(a), (b)] and 6H-SiC$(11\bar{2}0)$ substrate [(c), (d)]. (a), (c) were measured in x-ray incident geometry parallel to $[1\bar{1}00]$ direction, and (b), (d) perpendicular to $[1\bar{1}00]$ direction.

arc sec, suggesting noticeably small tilting around the [$11\bar{2}0$] direction. Figures 4(c) and 4(d) show the XRC profiles for the AlN epilayer grown on the 6H-SiC($11\bar{2}0$) substrate in those two geometries. The diffraction intensity in the x-ray incident geometry perpendicular to the [$1\bar{1}00$] direction [Fig. 4(d)] was considerably weak compared to that parallel to the [$1\bar{1}00$] direction [Fig. 4(c)]. Since there was no difference in ($11\bar{2}0$) diffraction for the 6H-SiC($11\bar{2}0$) substrate between those two geometries, this is probably attributed to many stacking faults or line defects expanding along the [$1\bar{1}00$] direction, which originated from the polytype mismatch of 2H-AlN/6H-SiC($11\bar{2}0$). From the results of the XRC measurements, the crystalline quality of the AlN epilayer grown on the 4H-SiC($11\bar{2}0$) substrate was much superior to that grown on the 6H-SiC($11\bar{2}0$) substrate owing to the polytype matching of 4H-AlN/4H-SiC($11\bar{2}0$).

The reason why the atomic template effect works well in AlN/4H-SiC($11\bar{2}0$), not in AlN/6H-SiC($11\bar{2}0$), has not been elucidated yet. In our speculation, 4H-AlN($11\bar{2}0$) can be grown on 4H-SiC($11\bar{2}0$) due to the similar structure of 2H (ABAB···) to 4H (AB$\underline{\text{C}}$B···), only one mismatch in every 4 monolayer (ML). On the other hand, 2H-AlN($11\bar{2}0$) is grown on 6H-SiC($11\bar{2}0$) because of more different structures between 2H (ABABAB···) and 6H AB$\underline{\text{CAC}}$B···), 3 mismatches in every 6 ML. It should be noted that the polytype of the AlN epilayer is strongly influenced by that of the SiC($11\bar{2}0$) substrate.

In conclusion, we have performed the growth of AlN on a 4H-SiC($11\bar{2}0$) substrate via PA–MBE, and the influence of substrate polytype on the crystalline structure of the AlN epilayer was investigated compared to 6H-SiC($11\bar{2}0$). 4H-AlN, has been grown on the 4H-SiC($11\bar{2}0$) substrate owing to the atomic-template effect, i.e., polytype replication. This is a completely different result from 2H-AlN growth on 6H-SiC($11\bar{2}0$), in which the polytype of substrate was not replicated. The FWHM of XRC ($11\bar{2}0$) diffraction for the 4H-AlN epilayer was as small as 90 arc sec, suggesting noticeably small tilting around the [$11\bar{2}0$] direction. The excellent crystalline quality is probably owing to the polytype matching between the 4H-AlN epilayer and the 4H-SiC substrate, which resulted in remarkable reduction of stacking faults or line defects at the interface. The high-quality 4H-AlN/4H-SiC($11\bar{2}0$) structure is expected to be a hopeful template to realize high-performance polarization-free nitride devices.

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[1] H. M. Ng, Appl. Phys. Lett. **80**, 4369 (2002).
[2] M. D. Craven, S. H. Lim, J. S. Speck, and S. P. DenBaars, Appl. Phys. Lett. **81**, 469 (2002).
[3] M. D. Craven, S. H. Lim, F. Wu, J. S. Speck, and S. P. DenBaars, Appl. Phys. Lett. **81**, 1201 (2002).
[4] N. Onojima, J. Suda, and H. Matsunami, Jpn. J. Appl. Phys., Part 2 **41**, L1348 (2002).