Polar Dependence of Threading Dislocation Density in GaN Films Grown by Metal-Organic Chemical Vapor Deposition *

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We investigate the threading dislocation (TD) density in N-polar and Ga-polar GaN films grown on sapphire substrates by metal-organic chemical vapor deposition. X-ray diffraction results reveal that the proportion of screw type TDs in N-polar GaN is much larger and the proportion of edge type TDs is much smaller than that in Ga-polar. Transmission electron microscope results show that the interface between the AlN nucleation layer and the GaN layer in N-polar films is smoother than that in Ga-polar films, which suggests different growth modes of GaN. This observation explains the encountered difference in screw and edge TD density. A model is proposed to explain this phenomenon.

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Because of the polar nature of the hexagonal GaN crystal when grown in the typical *c*-direction, the electrical and optical properties of GaN-based heterostructures and the properties of the crystal surface are strongly influenced by polarization effects.[1–6] The direction of the polarization field in N-polar GaN is opposite to that in group-Ⅲ-metal polar heterostructures, which enables the fabrication of devices with better performances.[7–10] For light-emitting diodes (LEDs), the N-polar structure is able to suppress the Stark effect in the quantum well so that the luminous efficiency is increased.[11] N-polar heterostructures also possess an inherent wide-bandgap AlGaN back barrier for electron confinement that reduces the short-channel effects. This leads to better off-state pinch-off characteristics as well as reduced on-state output conductance in high electron mobility transistors (HEMTs).[12–14]

Due to the lattice parameter mismatch and the difference in thermal expansion coefficient between GaN and sapphire substrates, threading dislocations (TDs) are intensely nucleated (density around 10^8–$10^{10}\,\mathrm{cm}^{-2}$). The effect of TDs on the performance of GaN-based devices is highly deleterious. In power devices, TDs would cause large reverse bias leakages, which can damage device operation. In optoelectronic devices, TDs will result in non-radiative recombination of carriers and decrease the internal quantum efficiency of optoelectronic devices.[15] It has been reported that the edge TDs are mostly produced in Ga-polar GaN films and the screw TDs are mostly created in N-polar GaN films.[16,17] Song *et al.*[18] studied epitaxial lateral overgrowth (ELOG) of N-polar GaN and found that most of the observed trends for N-polar ELOG are contrary to those reported for Ga-polar experiments. Due to the remarkable difference of TD characteristics between Ga-polar and N-polar GaN films, it is necessary to analyze the mechanisms for the formation and evolution of TDs in N-polar GaN film, so as to find more effective methods to reduce TD density and to obtain superior performance of N-polar GaN devices.

In this study, we investigate how the TDs density and typology in GaN films, grown by metal-organic chemical vapor deposition (MOCVD), are affected by the polar direction. The reasons of larger proportion of screw type TDs in N-polar GaN and larger proportion of edge type TDs in Ga-polar GaN are discussed.

N-polar and Ga-polar GaN films were grown on sapphire substrates in a low-pressure MOCVD reactor. H_2 was used as carrier gas and the reactor pressure was kept at 40 Torr. The substrates were first baked in H_2 at 1200℃ to clean any organic material and etch atomic-sized steps in the substrates. For the N-polar GaN sample, the substrate was then exposed to a high-temperature nitridation with a NH_3 flow of 150 mmol/min at 1100℃ for 3 min. The AlN nucleation layer was then deposited using a trimethylaluminum (TMAl) flow of 17 μmol/min and a NH_3 flow of 150 mmol/min at 1100℃ for 35 min. The temperature was then decreased to 1050℃ and the GaN layer was deposited using a triethyl-gallium (TEGa) flow of 100 μmol/min and a NH_3 flow of 130 mmol/min for 100 min. For the Ga-polar GaN sample, the growth parameters are the same, except that the NH_3 flow for high-temperature nitridation and AlN nucleation layer

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is 13 mmol/min. The total thickness of N-polar and Ga-polar epitaxial layers is estimated to be 1.55 μm and 1.52 μm, respectively. The surfaces of the as-deposited GaN layers were observed by an optical microscope. The microstructures of the samples were evaluated by x-ray diffraction (XRD) and transmission electron microscope (TEM) measurements.

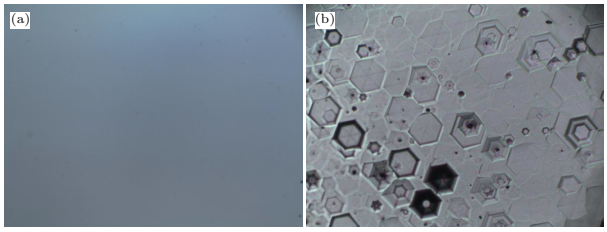

Fig. 1. Microscopic images of (a) Ga-polar and (b) N-polar GaN film surfaces.

As shown in Fig. 1(a), the Ga-polar GaN film exhibits a smooth surface. On the other hand, a rough surface with hexagonal hillocks is observed on the N-polar GaN film in Fig. 1(b). The appearance of hexagonal hillocks is a typical characteristic for the morphology of N-polar GaN surface.[19] The polarities of GaN films are also examined by wet etching. It has been reported that the relative stability of the AlN films depends on the chemical potentials of Al and N. Films having Al-polarity are expected to form under Al-rich conditions, while an N-rich deposition of AlN is expected to lead to a film with N-polarity, which is coherent with this study.[20]

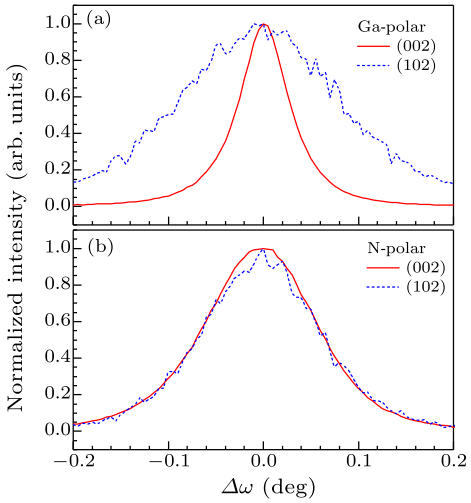

Fig. 2. XRD FWHMs of GaN samples with different polarities: (a) Ga-polar GaN, (b) N-polar GaN.

The structural properties of the GaN films are examined in Fig. 2 by recording the on-axis symmetric and off-axis symmetric skew of XRD rocking curves. The full width at half maximum (FWHM) of the symmetric (002) rocking curve correlates with the number of screw TDs. The off-axis (102) measured in a skew symmetric geometry is sensitive to the presence of pure edge TDs.[20] The FWHM of the rocking curves at the (002) and (102) planes of Ga-polar GaN sample are 229 arcsec and 705 arcsec, respectively, thus the TD density is estimated to be $1.1 \times 10^8\,\mathrm{cm}^{-2}$ for screw TDs and $2.6 \times 10^9\,\mathrm{cm}^{-2}$ for edge TDs.[21] The percentage fraction of screw type TDs is 3.8%. On the other side, for the N-polar GaN sample, the FWHM of the rocking curves at the (002) and (102) planes are 497 arcsec and 514 arcsec, respectively. Thus the TD densities are estimated to be $4.9 \times 10^8\,\mathrm{cm}^{-2}$ for screw TDs and $1.4 \times 10^9\,\mathrm{cm}^{-2}$ for edge TDs. The percentage fraction of screw type TDs in N-polar is 26.1%.

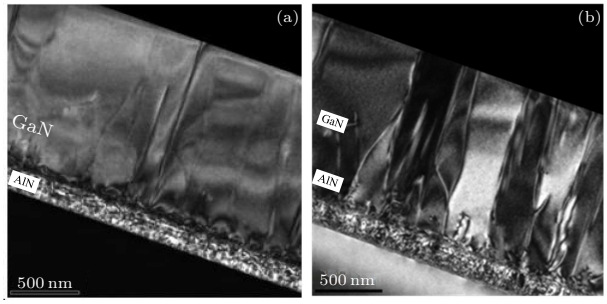

Fig. 3. Cross-sectional TEM images of the Ga-polar GaN film: (a) $g = [0002]$, and (b) $g = [11\bar{2}0]$.

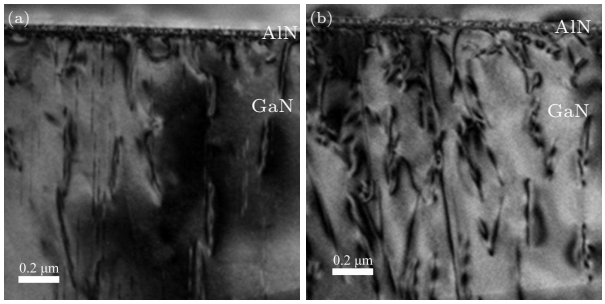

Fig. 4. Cross-sectional TEM images of the N-polar GaN film: (a) $g = [0002]$, and (b) $g = [11\bar{2}0]$.

To further investigate the features of TDs in the two samples, Tecnai 20 D522 S-Twin (TEM) has been used. The TEM samples were prepared by mechanical polishing and ion beam thinning up to cross sectional electron transparency. Cross-sectional TEM images with $g = [0002]$ and $g = [11\bar{2}0]$ of the Ga-polar GaN film are illustrated in Figs. 3(a) and 3(b), respectively. With $g = [0002]$, only pure screw dislocations and mixed dislocations are visible. With $g = [11\bar{2}0]$ only pure edge dislocations and mixed dislocations are observed. It is observed from Fig. 3(a) that only a few numbers of screw TDs in Ga-polar GaN propagate to the surface, since most screw TDs bend and annihilate during the initial growth of the GaN layer. It is obtained from Fig. 3(b) that a small part of the edge TDs bend and annihilate while most of them propagate to the surface. The edge TDs present an aggregated distribution in Ga-polar GaN film. Figure 4 shows the cross-sectional TEM images of a N-polar

GaN film. Plenty of screw TDs propagate to the surface with $g = [0002]$, while no TDs bending or annihilation is observed. Although the density of edge TDs in Fig. 4(b) is still high, the proportion of screw-type TDs is much larger, which is coherent with the results of the XRD measurement. The edge TDs present a random distribution in the N-polar GaN film.

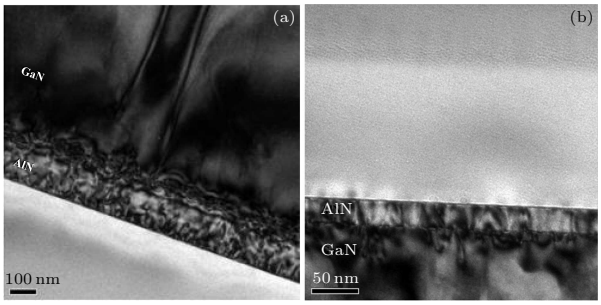

Fig. 5. Cross-sectional TEM images of the AlN nucleation layers with different polarities using $g = [0002]$: (a) Ga-polar GaN, (b) N-polar GaN.

Cross-sectional TEM images of AlN nucleation layers with different polarities using $g = [0002]$ are shown in Fig. 5. For the Ga-polar material in Fig. 5(a), the thickness of the AlN nucleation layer is about 180 nm. The interface between the AlN nucleation layer and the GaN epitaxial layer is irregular and coarse. In contrast, for the N-polar material in Fig. 5(b), the thickness of the AlN nucleation layer is about 30 nm. The interface between the AlN nucleation layer and GaN epitaxial layer is very clear, and the interface is quite smooth. The difference in thickness and surface morphology in the AlN nucleation layers with different polarities may be caused by different growth modes of AlN layers. Considering the atomic arrangements of AlN nucleation layers,[19] when aluminum atoms migrate to the surface of Al-polar AlN, they are likely to be captured by the nitrogen dangling bonds. The growth rate of the AlN nucleation layer along the (0001) direction is fast, which results in a thick AlN nucleation layer with rough surface. On the other hand, for the N-polar AlN nucleation layer, the number of dangling bonds pointing upwards is only 1/3 of that in the Al-polar AlN, thus few aluminum atoms are captured at the surface. As a result, the growth rate of the AlN nucleation layer along the (0001) direction is limited, which results in a thin and smooth AlN nucleation layer.

The variations of screw and edge TDs distributions in GaN layers with different polarities can be attributed to the growth mode during GaN initial growth. As shown in Fig. 6(a), for Ga-polar GaN films, the surface of AlN nucleation layer is quite rough, which results in the formation of GaN clusters on the AlN nucleation layer. In the initial process of the GaN bands growth, some TDs grow towards the top surface, while some TDs bend to the side of the clusters instead of propagating upwards. During the coalescence of the GaN layer, TDs arise at the boundaries of the GaN islands. It has been reported that most of the TDs generated at the clusters junctions are edge TDs.[22] Consequently, part of the screw and edge TDs bend while plenty of edge TDs arise at the boundaries of the GaN clusters. Thus edge TDs are dominant in Ga-polar GaN films, and edge TDs present an aggregated distribution in Ga-polar GaN film. For N-polar GaN in Fig. 6(b), the surface of AlN nucleation layer is rather smooth, thus the growth mode for N-polar GaN is layer by layer. The processes of GaN island growth and the following coalescence do not appear in the GaN layer, thus no edge TDs bending or migration to the boundaries occurs during the propagation of TDs in N-polar GaN films. The edge TDs present a random distribution in the N-polar GaN film. In consequence, the proportion of screw type TDs in N-polar films is much larger than that in Ga-polar films, while the proportion of edge TDs is smaller.

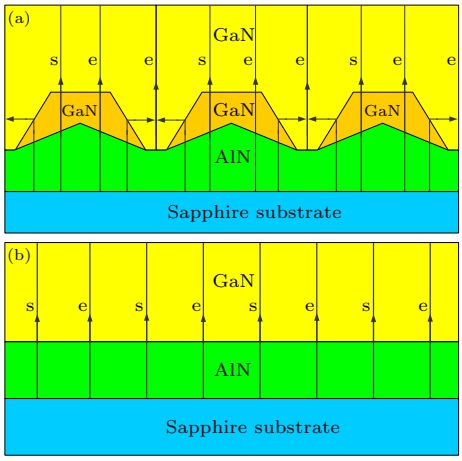

Fig. 6. Schematic diagrams of TDs propagation in (a) Ga-polar and (b) N-polar GaN films. Here s represents screw TD, and e represents edge TD, respectively.

In summary, we have studied the screw and edge TDs in N-polar and Ga-polar GaN films. The XRD results show that the proportions of screw type TDs in N-polar and Ga-polar films are 26.1% and 3.8%, respectively. The TEM measurements indicate that the surface of the AlN nucleation layer in N-polar films is smoother than that in Ga-polar films. For Ga-polar GaN, some screw and edge TDs bend during GaN clusters initial growth instead of propagating upwards, and plenty of edge TDs arise at the boundaries of the GaN islands, which makes edge TDs dominant in Ga-polar GaN films. In contrast, the growth mode for N-polar GaN is layer-by-layer, thus no TD bending or TD migration happens during the propagation of TDs in N-polar GaN films. In consequence, the proportion of screw type TDs in N-polar GaN films is significantly larger than that in Ga-polar ones. It is

expected that more effective methods to reduce TD density in N-polar GaN films are found and N-polar GaN devices with superior performance are obtained.

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