Core structures of the decorate edge dislocations in GaN epilayers

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ABSTRACT

Threading dislocations with edge components were investigated by a high-resolution transmission electron microscope in undoped GaN epilayers grown on Al_2O_3 substrates. Two types of core images were observed. One is a fully filled core with regular contraction and expansion of diffraction bright dots and the other is incompletely filled with one bright dot less and irregular contraction and expansion of bright dots. The impurities around the cores were detected to contain oxygen and carbon elements by energy-dispersive x-ray spectrometer. This suggests that both types of dislocations be decorated with impurities.

Keywords: dislocation, impurity, GaN.

1. INTRODUCTION

GaN and its related compound semiconductors are widely applied to fabricate high-brightness blue light emitting diodes, blue laser diodes, visible-blind detectors, high-temperature and high-power transistors after the breakthroughs in their epitaxial process. Most widely used substrate for their epitaxy is sapphire (Al_2O_3). However, the about 14% of lattice mismatch and the about 80% of thermal-expansion difference between the substrate and the epilayers usually bring about a high density of growth defects in the epilayers. Threading dislocations with edge components were dominant growth defects in the epilayers. Recently, the dislocations were predicted to be decorated with other defects.[1] However, the observed core images are the pure edge dislocations,[2] and investigation of the core images of the decorated dislocations was believed worthwhile.

In this work, the threading dislocations with edge components were investigated by a high-resolution transmission electron microscope (HREM) in undoped GaN epilayers grown on Al_2O_3 substrates. The core images were examined in detail and the core structure was sketched according to the projected charge density approximation. The impurities around the cores were detected by energy-dispersive x-ray spectrometer (EDS). The physical origins of the results are discussed.

2. EXPERIMENTAL

Samples used in this study were undoped GaN epilayers grown on (0001) sapphire substrates by metallorganic vapor phase epitaxy (MOVPE). The substrate was preheated to 1150℃ in a H_2 stream for 15 min. The substrate surface was then pre-nitridated in a H_2 and NH_3 mixed gas stream at 1150℃ for 3 min. A GaN buffer layer about 20 nm thick was deposited at 550℃. The temperature was then raised to 1050℃ and GaN was grown by feeding trimethylgallium and NH_3 gases into a reactor. As-grown epilayers were transparent with thickness of about 4 μm and a specular surface.

HREM specimens of about 3-mm diameter were cut out from the as-grown samples by a mini core picker. From the substrate side, the specimens were mechanically ground down to about 70-μm thickness and dimpled down to about 5-μm thickness. The specimens were thinned with Ar^+ ions at 1.5 kV and an incident angle of 2° from the GaN side and of 3° from the substrate side to reduce the influence of ion damage on the defect images. High-resolution observations of defects along the <0001> direction were carried out on a field emission HREM (JEOL JEM-2010F) operating at 200 keV. The impurities in GaN epilayers were analyzed on an energy-dispersive x-ray spectrometer (EDS) with the electron probe size of 0.7 nm and ultrathin window of Si (Li) detector in the field emission HREM.

3. RESULTS AND DISCUSSION

The end-on threading dislocations with edge components have densities of about 1×10^{11} cm^{-2} on the (0001) plane of

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GaN observed by HREM. The core images were measured in the thin regions where the weak-phase object approximation was hold.

The image structures of dislocations are characterized by two extra rows of diffraction bright dots in <11-20> directions that meet with an angle slightly larger than 60°, as a typical image shows in Fig. 1. The Burgers circuits around the dislocations were directly drawn in the lattice image and the Burgers vectors were measured to be 1/3<11-20> on the (0001) plane of GaN. The lattice distortions were determined by measuring the distances between the bright dots at cores and compared with the mean distance of the perfect regions in the images. The lattice in the Burgers vector directions contract and expanse above and below the intersection, respectively. The diffraction bright dots are distributed in broken lines in the Burgers vector directions. The broken lines fold at the mid-plane of the core perpendicular to the Burgers vector and project toward the contracted region. These cores are filled on the whole. Close examination revealed that the filling degree of the diffraction bright dots at the intersection is different and can be classified into two types. Type A is fully filled with a bright dot at the met position, as shown in Fig. 1(a). Type B is incompletely filled with the bright dot missing at the intersection, as shown in Fig. 1(b). We examined several tens of the cores, and found type A and B account for about 90 and 10 percent, respectively. The lattice distortions of type A and B were averaged. For type A, the mean contraction and expansion are 6 (±5) % and 13 (±5) % just above and below the intersection in the <11-20> directions parallel to the Burgers vectors. The mean distances between two nearby bright dots in other two <11-20> directions at the cores are the same as those of perfect regions within the error limit. For type B, the mean contraction and expansion are 12 (±10) % and 19 (±10) % just above and below the intersection in the <11-20> directions parallel to the Burgers vectors. The distances between two nearby bright dots arranged in other two <11-20> directions vary from core to core. Most of them contract and expanse above and below the intersection, respectively.

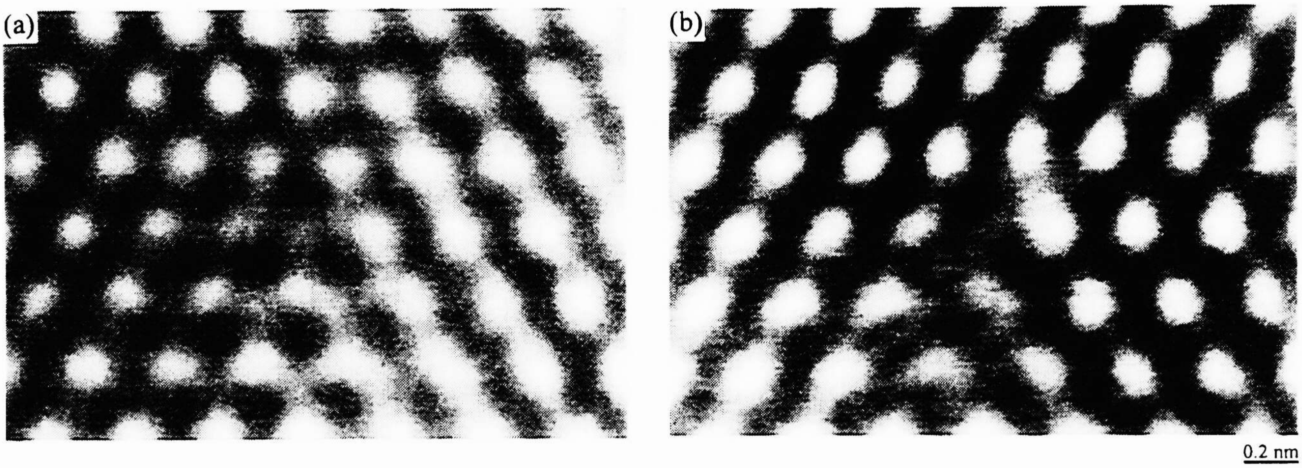

Fig. 1. Typical core images of type A (a) and type B (b) threading dislocations with edge components observed with the primary beam energy of 200 keV along <0001> direction of GaN.

The core structure projected along the <0001> direction was sketched according to the projected charge density approximation in which the obtained high-resolution image represents the specimen projected total charge density.[3] This approximation predicts an image dark in the regions where a large number of atoms forming columns in the electron beam direction. The bright regions are therefore interpreted as the tunnels seen in <0001> projections of GaN. The extra bright dot at the intersection of type A is unlikely to be caused by the distortions of two nearby bright dots arranged in the Burgers vector direction due to the disturbance of a stress field to atomic column shapes.[4] Therefore, we simply interpret the extra bright dot as four-fold ring, as shown in Fig. 2(a), which is favorable for dispelling surface energy caused by the column of three-fold coordinated atoms. On the contrary, the type B image is characterized without the bright dot, which indicates there are more atomic columns at the core. It has been shown previously that the threading dislocations have a relaxed core.[2] In the relaxed core, the distance contractions of the three atomic columns above the intersection are about 15%, which may form a column with a large number of charge carriers and hinders the electron beam to tunnel through and results in the bright dot disappearance. For this reason, the type B image is related to the relaxed core with one column of three-fold coordinated atoms, as shown in Fig. 2(b). However, the degrees of the contraction and expansion of the type B image vary from core to core. This variation must arise from slightly different core structures.

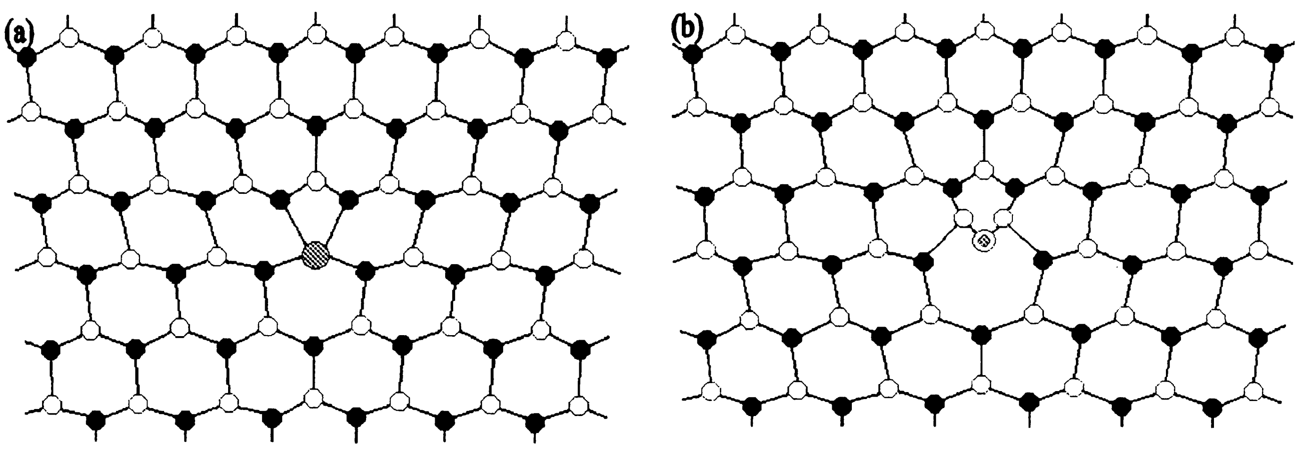

Fig. 2. Sketch of the core structure of type A (a) and type B (b). The open and dark solid circles represent atomic columns comprising alternating Ga and N atoms. The grey solid circle represents an atomic column where impurity is likely to precipitate.

It is known that smaller and larger atoms are preferably substitute for host atoms in contraction and expansion lattices, respectively, and form decorated dislocations. To understand the precipitation, the impurities around the cores were detected by EDS. The EDS spectra around both types of cores exhibit the strong characteristic x-rays of Ga and N elements, as typical spectrum shown in Fig. 3. On the high energy side of the N characteristic x-ray, the characteristic x-ray of O element is recognizable. On the low energy side of N characteristic x-ray, a weak and broad shoulder is visible, which seems attributable to the very low density of the C impurity. Since the electron probe size of 0.7 nm covered several diffraction bright dots, it is impossible to determine the substitutional sites of impurities at the cores. However, theoretical calculations showed that substitutional O onto the N site has an outward relaxation of the neighboring host atoms and a much lower formation energy.[5] This is favorable for substitutional O onto N site in the expansion lattice below the intersection of the two extra rows. Furthermore, one remaining valence electron of the substitutional O might combine with the lone bond of the three-fold coordinated atoms of the relaxed core and form the core structure of type A. This further supports the core structure of type A. For type B core, local-density-functional calculations shows that three kinds of gallium vacancy-oxygen defect complexes are most favorable to trap in threefold coordinated position and form new distorted configurations in the stress field of threading-edge dislocations.[1] This suggests that the threading-edge dislocation decorated with gallium vacancy-oxygen defect complexes is dominantly responsible for type B image and the different decorated defects of $(V_{Ga}\text{-}O_N)^{2-}$, $(V_{Ga}\text{-}O_N)^{-}$ or $V_{Ga}\text{-}(O_N)_3$ result in the variation of type B image. On the other hand, C substituted onto both N and Ga sites were calculated to have an inward relaxation of the neighboring host atoms.[6] From the standpoint of the elastic strain energy release, this is beneficial for C substituted onto Ga site in the contraction lattices. Particularly, type B core has a threefold coordinated atomic column and contracts more obviously. These are favorable for C substituted onto Ga site in threefold coordinated atomic column. On the basis of above results, we suggest that both types of dislocations be decorated with defects.

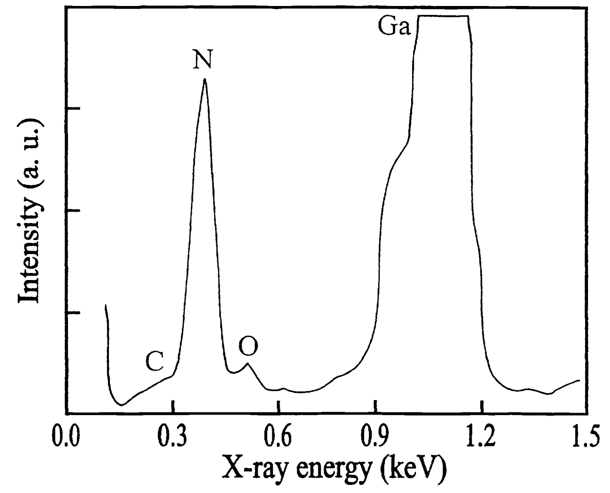

Fig. 3. EDS spectrum around the core measured by an electron beam with spot size of 0.7 nm.

4. CONCLUSIONS

Two types of core images of threading dislocations were observed in undoped GaN epilayers grown on Al_2O_3 substrates. Type A is a fully filled core with regular contraction and expansion of diffraction bright dots and type B is incompletely filled with one bright dot less and irregular contraction and expansion of bright dots. Their core structures projected along the <0001> directions were sketched according to the projected charge density approximation. The impurities around the cores were detected to contain O and C elements. This suggests that both types of dislocations be decorated with impurities.

5. ACKNOWLEDGEMENTS

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