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The Relationship between the Bending Direction and Burgers Vector of Threading Dislocations at a Coherent Heterointerface in AlGaN/AlN Layers

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Transmission electron microscope analysis of microstructure in AlGaN/AlN thin layers was performed to investigate the behavior of threading dislocations (TDs). The absolute values of the Burgers vectors (***B***) of TDs were determined from the change in number of thickness fringes in the weak-beam dark-field images. In the AlGaN/AlN thin layers grown on α-Al_2O_3 (0001) substrate, there were a lot of TDs propagating along [0001] with ***B***=***a***, where ***a*** is the corresponding axis vector. These TDs were observed to bend at the hetero-interface of AlGaN/AlN. It was confirmed that the bending direction is normal to ***B*** and that the extra half plane associated with the TD decreases in area by the bending. Precise measurement of the in-plane lattice dimensions showed that there exists a compressive strain in AlGaN on the hetero-interface. These results revealed that control of internal stress is an important factor to govern the behavior of TDs.

Introduction

Aluminum gallium nitride ($Al_xGa_{1-x}N$, AlGaN) is a promising material for light-emitting diodes and laser diodes of a short wavelength range including ultraviolet that is essential to white illumination. It is very hard, however, to fabricate AlGaN thin films of a good quality. It was reported that crack-free AlGaN films were fabricated successfully on a GaN template with an AlN interlayer deposited at a rather low temperature or an LT-AlN-IL [1]. One of the present authors showed that the formation and annihilation of dislocations play a role in reduction of stress originated from the difference in lattice parameter between the layers of different compositions [2]. This indicates that the analysis of dislocations is quite important to control the microstructures with hetero-interfaces. In this work, transmission electron microscope (TEM) analysis was carried out for threading dislocations (TDs) near the hetero-interface of AlGaN/AlN to clarify the relationship between the morphology of TDs and the internal stress.

Experimental

$Al_xGa_{1-x}N$ layers with almost equiatomic compositions on an AlN/α-Al_2O_3(0001) template were prepared by a conventional metal-organic vapor-phase epitaxy (MOVPE) method using trimethyl-Al, trimethyl-Ga and ammonia in a carrier gas of hydrogen. Thin foil specimens for cross section and plan-view TEM observations were made by using a focused ion beam (FIB) mill with a microsampling unit and an argon ion mill. Observation was carried out with a Tecnai-F20 microscope operated at 200 kV.

Results and Discussion

Fig. 1 shows cross section dark-field (DF) images of AlGaN/AlN/α-Al_2O_3(0001) taken with a diffraction vector of $g=01\bar{1}0$ and 0002, respectively. A lot of TDs are generated at the interface of AlN/α-Al_2O_3(0001) and propagate upwards along [0001]. It is clearly seen that most of them have a Burgers vector (***B***) of ***a***, where ***a*** is the corresponding crystal-axis vector, so that they disappear from the DF image taken with g=0002. The TDs of ***a***-type propagate into the AlN layer with bending at the interface of AlGaN/AlN.

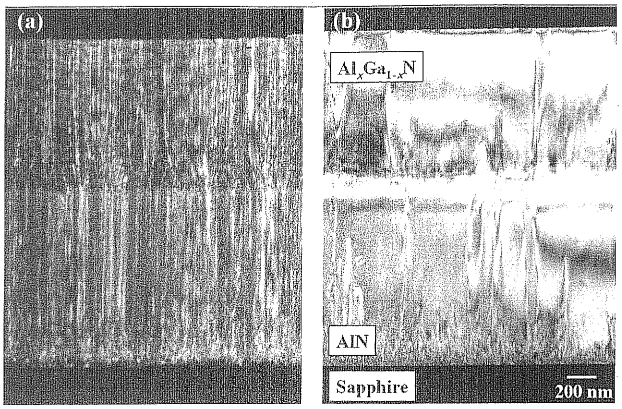

Fig. 1 Cross sectional DF images of $Al_xGa_{1-x}N(x=0.5)/AlN/\alpha\text{-}Al_2O_3$
(a) $g=01\bar{1}0$ (b) $g=0002$

Fig. 2 shows a plan-view bright field (BF) image and a plan-view DF image of the AlGaN layer in the area just above the interface of AlGaN/AlN. In the BF image taken with a [0001] zone axis illumination, TDs are seen as lines along three directions of $<1\bar{1}00>$, which reflects that these TDs are inclined toward these directions. As seen in the two-beam DF image taken with $g=\bar{1}100$, TDs along the direction of $[\bar{1}100]$ are out of contrast. It is revealed from the fact that the inclining directions of TDs, ***p***, are normal to their Burgers vectors ***B***. It should be noted that the direction of inclination ***p*** does not lie on the slip-plane of the TD. If the inclination is attributed to internal stress, an extra half-plane is there under the bending TD in the region with compressive stress and vice versa. Therefore, the sign of Burgers vector becomes essential in explanation of morphology of TDs. In this work, the absolute values of Burgers vectors were determined from the change in thickness contours in a weak-beam DF image [3,4]. In this determination, it is important to avoid unnecessary confusion due to the 180° rotation of image, the side-reverse of negative films (or a CCD camera) and others. Fig. 3 shows an example of cross sectional weak-beam DF images. It is noted that the sense of change in the number of thickness contour around TDs marked with 'A' and 'B' is different from each other in spite of the same directions of inclination of these TDs. This seems as if the TDs have a Burgers of a reverse sign, but this is not the case. Let the illumination be along $[01\bar{1}0]$ and the diffraction vector be $g=2\bar{1}\bar{1}0$, the TDs are thought to be inclined toward $p=[10\bar{1}0]$ and $[1\bar{1}00]$ and have the Burgers vector of $B=[1\bar{2}10]/3$ and $[\bar{1}\bar{1}20]/3$, respectively, and in turn, the sense of change in number of thickness contours is different since gB=1 and -1. The absolute values of ***B*** and the inclining directions p were also confirmed by the weak-beam DF image method and the stereographical method after rotating the thin foil specimen along [0001] by ±30° The result of $\boldsymbol{B}$ and p leads to the situation where there is an extra half-plane under both of the inclined TDs.

We examined the axis-ratios c/a for local areas in the AlN and AlGaN layers from the selected-area (SA) electron diffraction patterns. It has been confirmed that the relative changes in c/a can be obtained in accuracy better than 0.1%. Fig. 4 shows the variation in reciprocal of c/a as a function of the distance from the interface of AlN/ α-Al_2O_3 It is seen that there are compressive stresses in the lower region of AlGaN layer. It is very natural that the sense of stress is of compression in the AlGaN layer since the lattice dimension a of AlGaN is larger than that of AlN. From these results, it can be concluded that the bending of TDs at the heterointerface of AlGaN/AlN is attributed to reduction of internal compressive stress due the difference in in-plane lattice dimension between the AlGaN and AlN layers. In this connection, Romanov and Speck [5] suggested a similar mechanism of bending of TDs in terms of stress.

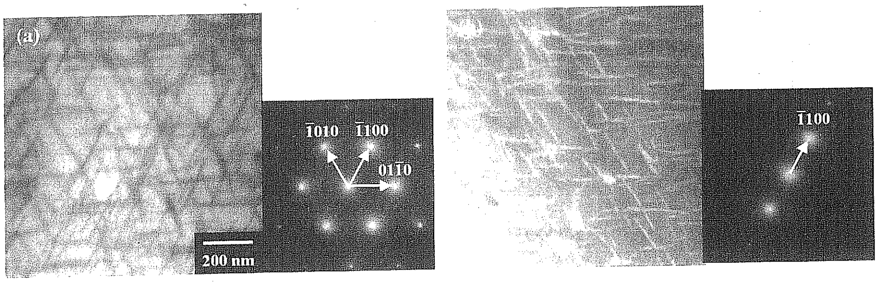

Fig. 2 Plan view images of AlGaN just above the interfacc of AlGaN/AlN
(a) BF image with [0001] zone axis illumination
(b) Two-beam DF image with $g=\bar{1}100$

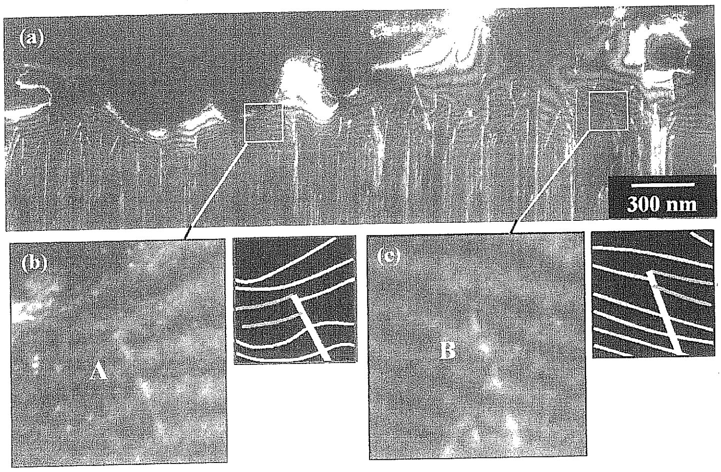

Fig. 3 Weak-beam DF image of AlGaN
(a) Wide area observation
(b)(c) Enlarged images of the regions marked with a square in (a)

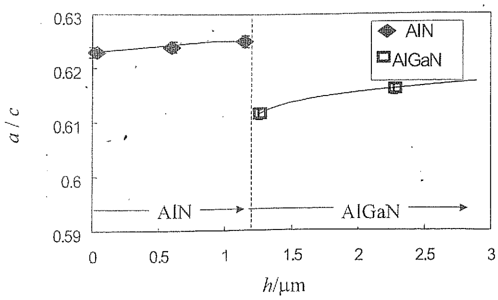

Fig. 4 Variation in c/a of AlN and $Al_xGa_{1-x}N$(x=0.5) as a function of the distance h from the interface of AlN/α-Al_2O_3

Summary

TEM analysis was carried out to investigate the origin of bending of TDs at the heterointerface of AlGaN/AlN, and the following results were drawn.

(1) TDs are inclined toward one of $<1\bar{1}00>$ direction.
(2) The direction of inclination is normal to the Burgers vector of each TD.
(3) The sense of Burgers vector leads to the situation where there is an extra half plane under the inclined TD.
(4) The bending of TDs is attributed to reduction of internal stress above the interface.

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