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Microstructural characteristics of GaN/AlN thin films grown on a Si (110) substrate by molecular beam epitaxy: Transmission electron microscopy study

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The growth of III-nitride thin films with a high quality including few defects is essentially required for many applications, such as optical devices, high frequency devices, and high power devices [1, 2]. The III-nitride compound semiconductors are a tetrahedrally coordinated binary compounds, found in either cubic zinc-blende (ZB) or hexagonal wurtzite (WZ) structures [3]. The two structures, ZB and WZ, differ in the relative handedness of the fourth interatomic bond along the (111) chain. The layer stacking sequence for WZ is ABABABA…, and that of ZB is ABCABCA…, along (111), respectively [3, 4]. The epitaxial growth of AlN and GaN thin films on silicon (Si) substrates is very attractive, as it has several advantages, such as high quality and large area, compared with compound substrates. In addition, nitride-on-silicon structures afford the possibility of an excellent candidates for unique design architectures and for creating devices for high-power applications. Therefore, much effort has been concentrated on the growth of AlN and GaN layers on Si substrates [5-7].

For the epitaxial growth of nitride thin films, a Si (110) wafer has begun to attract attention as a substrate, due to its interesting interface structure [5, 8, 9]. When nitrides are grown on a Si (110) substrate, the orientation relationship between the GaN and AlN and the Si is $(1100)_{GaN, AlN}$ // $(001)_{Si}$ and $[0001]_{GaN, AlN}$ // $[110]_{Si}$;there is an anisotropic lattice mismatch; the lattice mismatch along the $[1100]_{GaN, AlN}$ //$[001]_{Si}$ direction is small, close to 0 %, and the mismatch along the $[1120]_{GaN, AlN}$ //$[110]_{Si}$ direction is huge, approximately 20 %. This anisotropic lattice mismatch may contribute to particular growth behavior and defect structure in the nitride thin films.

The main purpose of this study was to understand microstructural properties, such as the atomic structure, dislocation distribution, and strain behaviors, of GaN/AlN structures grown on Si (110) substrates. The microstructural properties of the GaN/AlN structures were studied in detail using TEM. Specifically, the interface structures between the GaN, AlN and the substrate and the dislocation behavior at the interfaces were detailedly studied using bright-field and dark-field (BF and DF) TEM images taken under two-beam conditions and HRTEM micrographs. In order to study the strain behavior at the interface, geometrical phase analysis (GPA) was conducted using the GPA for Gatan DigitalMicrograph program from HREM Research Inc.

The schematic diagram of GaN/AlN/Si (110) structures was shown in Fig. 1(a). The analysis of the SAED patterns in Fig. 1(b) indicates that the orientation relationship between the WZ structure of the AlN and the Si(110) substrate was $[1120]_{GaN/AlN}$//$[110]_{Si}$ and $(0001)_{GaN, AlN}$//$(110)_{Si}$.

The BF and DF TEM images in Fig. 2 correspond to g = [0002] of the WZ structure of GaN and AlN, where the specimen has been tilted slightly from the [1120] zone axis around a tilting axis perpendicular to the growth surface. By applying the invisibility criterion, $g{\cdot}b=0$, where g is a diffraction vector and b is a dislocation Burgers vector, it is likely that the dislocations in Figs. 2(a) and 2(b) have a Burgers vector vertical to the interface, most probably b = [0002] of the WZ structure, i.e. they are of pure screw-type because the line direction ξ of a dislocation for c-oriented GaN is paralleled to the [0002] growth direction. The type of dislocation was determined compare with other obtained BF and DF images from g = [1100] of the WZ structure of GaN and AlN. The dislocations in the thick AlN layer were mainly generated at the thick-AlN/buffer-GaN interface and a few screw-type dislocations were propagated to the AlN surface.

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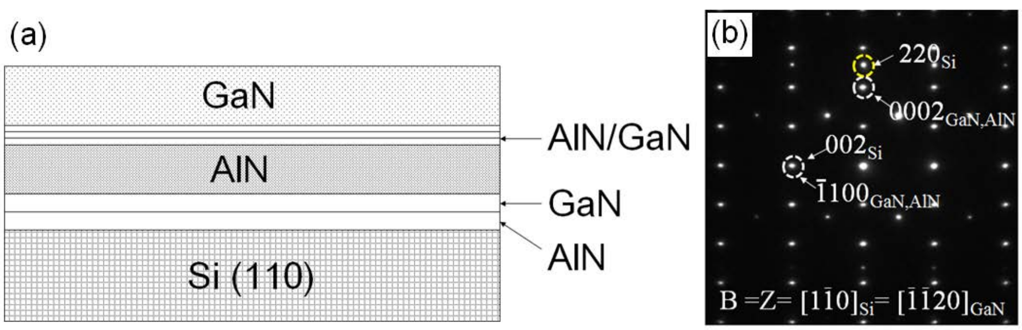

FIG. 1. (a) Schematic diagram of GaN/AlN/Si (110) structure. (b) SAED pattern taken along the $[\bar{1}\bar{1}20]_{GaN, AlN}$//$[1\bar{1}0]_{Si}$ zone axes of the GaN/AlN thin film grown on a Si (110) substrate.

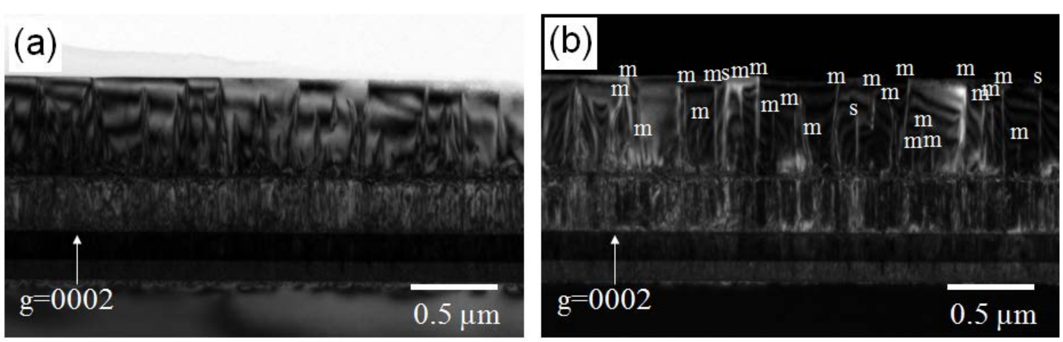

FIG. 2. (a) BF and (b) DF TEM images taken from the cross-section specimen for the GaN/AlN thin film using two-beam condition: g = 0002 [zone axis, $_z$ = $[1120]_{AlN}$//$[110]_{Si}$].

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