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Microstructural characteristics of AlN thin layers grown on Si(110) substrates by molecular beam epitaxy: Transmission electron microscopy study

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ABSTRACT

The microstructural properties of an aluminum nitride (AlN) layer grown on a silicon (Si(110)) substrate were studied in detail using transmission electron microscope techniques to determine atomic structure and dislocation behavior. AlN islands elongated along the $[11\bar{2}0]_{AlN}//[\bar{1}10]_{Si}$ direction were observed at the initial growth stage on the Si(110) substrate. The threading dislocations with a Burgers vector vertical to the interface, most probably $b_e = [0001]$ of the wurtzite structure, were frequently observed in the AlN thin film. Due to anisotropic biaxial strain distributions, two different atomic structure behaviors were observed along the two in-plane directions; a coherent interface was observed along the $[11\bar{2}0]_{AlN}//[\bar{1}10]_{Si}$ direction and a semicoherent interface, including periodic extra-half planes, was observed along the $[\bar{1}100]_{AlN}//[001]_{Si}$ direction. The extra-half planes were observed at approximately two monolayers above the interface, and not at the exact interface.

1. Introduction

The epitaxial growth of III-nitride compound semiconductors on silicon (Si) substrates is very attractive, as it has several advantages, including high quality, large area, and low cost, compared with substrates of compound semiconductors. In addition, it affords the possibility of large-scale integration of compound semiconductors for use in optical and electronic devices. In particular, nitride-on-silicon structures are considered to be excellent candidates for unique design architectures and for creating devices for high-power applications. Therefore, a great deal of effort has been concentrated on growing compound semiconductors on Si substrates [1–6].

However, there are several fundamental problems associated with growing nitride compound semiconductors on Si. First, the large difference in lattice constants and thermal expansion coefficients between layers and substrates can introduce misfit dislocations at the interface and cause stress in the epitaxial films. Second, the growth of polar compounds on non-polar substrates can lead to defect formation, such as an antiphase domain boundary. Despite these problems, epitaxial nitrides have been grown on Si substrates [7–10]. Among binary- and ternary-nitride semiconductors, aluminum nitride (AlN) has played a key role in epitaxial growth as nucleation and buffer layers on Si substrates. AlN is a tetrahedrally coordinated binary compound semiconductor of the $A^N B^{8-N}$ type, found in either hexagonal wurtzite (WZ) or cubic zinc-blende (ZB) structures [11]. Most studies on the epitaxial growth of nitrides on Si substrates have been carried out on (111) and (100) Si wafers. Although the percentage of lattice mismatches reached 16.9% for gallium nitride (GaN) and 19% for AlN, and although a number of dislocations were introduced, Si(111) was selected as the substrate for the epitaxial growth of nitrides because it is always favored due to its three-fold symmetry at the surface, which provides good rotational matching for the six-fold symmetry of the wurtzite structure of nitrides [4]. Si(001) has also been used to grow nitrides because of a possible integration of nitride devices with Si technology, despite four-fold symmetry and surface reconstruction [4,12]. However, the transport and microstructural properties of nitrides grown on Si(111) and Si(001) substrates were not good enough for use in electrical and optical devices. The large lattice mismatches between nitrides and Si(111) substrates causes a high rate of dislocation density in the nitride layers, and growing nitrides on Si(001) substrates is a challenging issue due to the lattice plane orientation and the different types of surface reconstructions.

Recently, Si(110), one of the surface orientations used in silicon technology, has begun to attract attention as a substrate for the epitaxial growth of nitrides, due to its interesting interface structure [1,4,13]. Fig. 1 shows the orientation relationship between AlN and Si when the growth direction of the WZ AlN grown on Si(110) is the $[0001]_{AlN}$ direction. The Si(110) plane displays mirror

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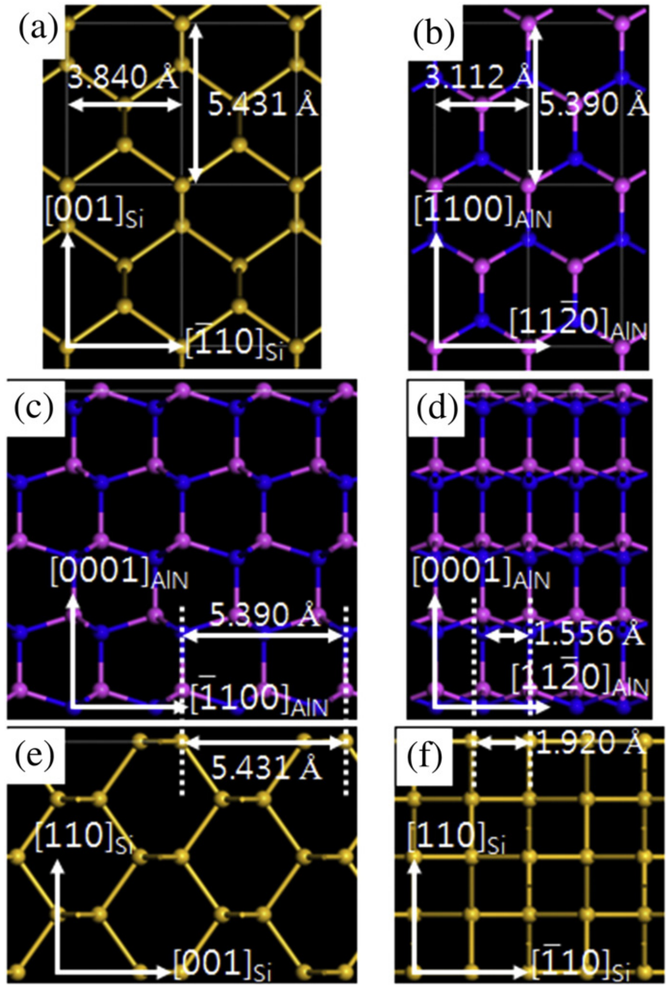

Fig. 1. Atomic arrangements of AlN on Si(110). (a) and (b) Projection along the [110] direction of Si and the [0001] direction of AlN, (c) and (d) Projection along the [11$\bar{2}$0] and [1$\bar{1}$00] directions of AlN, (e) and (f) Projection along the [$\bar{1}$10] and [00$\bar{1}$] directions of Si, respectively.

symmetry, and there is an anisotropic lattice mismatch; the lattice mismatch along the $[\bar{1}100]_{AlN}//[001]_{Si}$ direction is −0.8%, and the mismatch along the $[11\bar{2}0]_{AlN}//[\bar{1}10]_{Si}$ direction is −19.0%. The close lattice match along the $[\bar{1}100]_{AlN}//[001]_{Si}$ direction promotes faster growth along the particular crystal orientation—the $[11\bar{2}0]_{AlN}//[\bar{1}10]_{Si}$ direction. These particular characteristics may contribute to a higher crystalline quality of the nitrides.

However, until now, there have been few studies on the growth of nitride compound semiconductors on Si(110) substrates from a microstructural point of view. In this work, the microstructural properties of AlN thin films grown on Si(110) have been characterized using various transmission electron microscopy (TEM) techniques. The main purpose of this study was to understand the atomic structure, dislocation distribution, and strain behaviors of AlN structures grown on Si(110) substrates by molecular beam epitaxy (MBE). Insight gained at the microscopic level regarding how an AlN layer grows at the interface is essential for the growth of high-quality thin films for various applications.

2. Experimental

Undoped AlN layers were grown on Si(110) substrates using an MBE system equipped with a nitrogen radio frequency (RF) plasma source, an ammonia (NH_3) supply, and a standard effusion cell for Al. The Si substrate was chemically etched to remove the oxide layer and to produce a hydrogen-terminated surface. The chemically etched substrates were introduced into the vacuum chamber immediately after the wet process. A deoxidation procedure was used to prepare a reconstructed Si surface. The clean surface of the substrate was proved by the reflection high energy electron diffraction (RHEED) transition from the 16 × 2 to the 1 × 1 patterns. An AlN layer was grown using a nitrogen RF plasma source. The Si substrate was exposed to the nitrogen plasma for 20 s at 700 °C, followed by a rapid annealing process at 820°C for 10 s. The temperature was decreased to 650 °C to deposit the Al, and then the AlN layer was grown at 940 °C under a 200 W RF power and a 2 sccm flow of N_2. A streaky RHEED pattern was observed all along the growth of a 50-nm thick AlN layer.

The microstructural properties of the AlN structures were studied in detail using TEM. The specimens were prepared using standard methods of mechanical grinding and argon (Ar)-ion beam milling. A plasma treatment was conducted before loading the specimen to remove surface contamination and to avoid electron beam damage during TEM. Bright-field TEM (BFTEM) images, selected-area electron diffraction (SAED) patterns, and high-resolution TEM (HRTEM) micrographs were collected using an FEI F30 microscope operating at 300 kV. Specifically, the detailed interface structures between the AlN and the substrate were studied using TEM techniques. 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 dimension for the GPA analysis was 512 × 512 pixels. The HRTEM micrographs used for GPA were filtered through the DigitalMicrograph program.

3. Results and discussion

Fig. 2 shows representative plane-view TEM images taken from the very thin AlN structure grown on a Si(110) substrate to study the initial growth stage. The BFTEM image, taken under a multibeam condition, shows AlN islands grown through the merged 3-dimensional island growth mode. The AlN islands shown in Fig. 2(a) and (b) have elongated and merged shapes along the [11$\bar{2}$0] direction of AlN and the [$\bar{1}$10] direction of Si. Fig. 1(b) shows straight lines aligned vertically from the elongated direction in the island, which must be paralleled Moiré patterns caused by the superimposed lattice planes of the AlN and the Si. In the HRTEM micrograph shown in Fig. 1(c), the interval of the Moiré fringes is approximated to 16.10 Å. In the paralleled Moiré fringes, the interval, $d_{\Delta g^*}$, is determined as follows:

$$d_{\Delta g^*} = \frac{d_{h_1k_1l_1} d_{h_2k_2l_2}}{d_{h_1k_1l_1} - d_{h_2k_2l_2}} \quad (1)$$

where $d_{h_1k_1l_1}$ and $d_{h_2k_2l_2}$ are the interplanar spacings that contribute to the formation of the Moiré pattern.

In Fig. 2(c), the lattice planes related to the Moiré patterns are the {11$\bar{2}$0} planes from the AlN and the {$\bar{2}$20} planes from the Si, which is also consistent with the orientation relationship described in Fig. 1. Using Eq. (1), the interval between the Moire fringes is 16.41 Å, because the lattice planes related to the formation of the Moiré fringe are the $(11\bar{2}0)_{AlN}$ and the $(\bar{2}20)_{Si}$ planes, and this is approximated to the experimentally observed value (~16.10. Å). In the SAED pattern shown in Fig. 2(d), the orientation relationship between the AlN and the Si is $(\bar{1}100)_{AlN}$ // $(001)_{Si}$ and $[0001]_{AlN}$ // $[110]_{Si}$. The SAED pattern shows satellite spots along the [$\bar{2}$20] direction of Si while the spots along the [002] direction of Si are free from additional spots. The satellite spots along the [$\bar{2}$20] direction have two different origins: the first one, related to the spot indicated by the arrow, is the deposited AlN, and the other, indicated by the dotted circle, is the overlapping of the lattice planes of the AlN and the Si, which has the same meaning as the Moiré fringes shown in Fig. 2(b) and (c).