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Mechanism of defects formation and surface smoothening of AlN films grown on Si(111) by an NH_3 pulsed-flow method

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In this paper, we investigate the growth of AlN films on Si (111) substrate by an NH_3 pulsed-flow method. Compared with AlN films grown with a continuous NH_3 flow, the AlN films grown by the pulsed NH_3 flow method shows a smoother surface, and quasi-two-dimensional growth is achieved. But the (0002) and (10–12) FWHM show that the crystal quality of AlN films grown by the NH_3 pulsed-flow method is slightly deteriorated, indicating that more defects are formed. The defects formation and surface smoothening mechanisms are discussed.

1. Introduction

III-nitride materials have been extensively used in high frequency electronics and optoelectronic devices. In particular, AlN film and its ternary alloys, which possess direct wide band gap as well as good thermal and chemical stability, extend the application of group-III nitrides to high temperature and high power field [1]. Recently, the growth of group-III nitrides on Si has attracted much attention, since Si substrate has many advantages such as large size, low cost and good thermal conductivity [2]. But due to the outdiffusion of Si, it is difficult to grow GaN or InN directly on Si substrate [3]. AlN has been widely used as a seed layer for the growth of GaN or InGaN. And a high-quality AlN epitaxial layer is necessary for the subsequent growth of high quality GaN film.

However, there are several fundamental problems associated with growing AlN films on Si. First, the large difference in lattice constants and thermal expansion coefficients between AlN and Si (111) can introduce misfit dislocations at the interface and cause stress in the epitaxial films. Second, the low Al adatom mobility on Si is also an important issue with respect to a fast coalescence of the initial AlN crystallites and their size. Third, the gas-phase parasitic reactions between TMAl and NH_3 deteriorate the quality of AlN greatly [4]. To overcome these problems, high growth temperature over 1300 °C [5] and low growth pressures of 30–50 Torr [6] have been employed to enhance the surface migration of Al adatom species and to suppress parasitic gas-phase reaction between TMAl and ammonia. However, in many cases, it is very hard to increase the growth temperature above 1300 °C, because it is beyond the capability of the heating element of the reactor system, especially for resistance heating. As reported by Duan Huantao et al. [7] and Fawang Yan et al. [8], the NH_3 pulsed-flow method can

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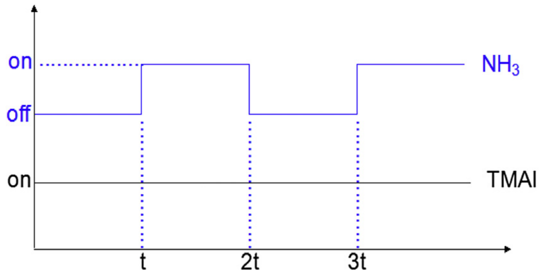

Fig. 1. Gas flow sequence used in NH_3 pulse-flow growth.

effectively increase the mobility of Al adatom and suppress the parasitic reactions between TMAl and NH_3, which can greatly improve the surface morphology and crystal quality of AlN films. But the NH_3 pulsed-flow method has hardly ever been used for the growth on AlN films on Si (111). In this work, 0.2-μm-thick AlN films are directly grown on Si(111) substrates using either a continuous or pulsed NH_3 flow process. The surface morphology, crystal quality and stress state are investigated.

2. Experimental

AlN films were grown on Si(111) substrates by metalorganic chemical vapor deposition (MOCVD) in THOMAS SWAN 19 × 2 GaN reactor system. Trimethylaluminum (TMAl) and ammonia (NH_3) were used as precursors and H_2 was used as carrier gas. The Si substrate was chemically cleaned by a typical RCA process and was etched in a 2.5% HF solution for 1 min prior to growth. The gas flow sequences used for the pulsed NH_3 flow process are shown in Fig. 1. The duration and interruption time of the supply of NH_3 gas flow are the same. Three samples were investigated. Sample A was grown with a continuous NH_3 supply. Sample B and sample C were grown with a pulsed NH_3 flow and the interruption duration of NH_3 were 9s and 15s respectively. For the integral evaluation of the crystalline quality we applied X-ray diffraction (HRXRD) using a Bruker D8 Discovery system. Rocking curves for the (0002) and (10−12) AlN reflection were acquired for all samples. The surface roughness of the layers was evaluated by atomic force microscopy (AFM) and Scanning Electron Microscopy (SEM). The stress state and curvature of AlN films are studied by Raman spectra and surface profilometer respectively.

3. Results and discussions

Fig. 2 shows the SEM images of AlN samples grown under different conditions. Sample A depicts porous structure while others show rice-like grain structure. Compared to sample C, the relative area of flat surface of sample B increases and the density of protrusions on the surface decreased as the NH_3 interruption duration changed from 15s to 9s. Fig. 3 shows the atomic force microscope (AFM) images. The surface morphology of sample B is much smoother and exhibits a quasi-two-dimensional growth mode with a root mean square (RMS) value of 2.08 nm, which indicates that the AlN seed layer has began to coalesce and preserves a more smooth growth front unaffected by the problems of melt-back etching. Others all exhibit a lot of small protrusions on the surface which are consistent with the results of Fig. 1.

Adatom diffusion is considered to be responsible for surface morphology. For mass transport on the surface, the surface diffusion length Ls is expressed as:

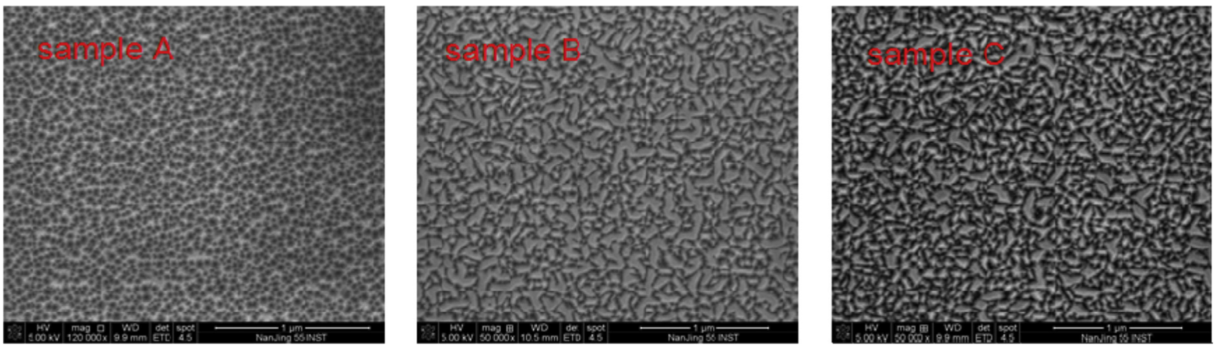

Fig. 2. SEM images of the surfaces of sample A, sample B, and sample C.

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