Expansion of lattice constants of aluminum nitride thin film prepared on sapphire substrate by ECR plasma sputtering method

Satoru Kaneko1,6, Hironori Torii2, Takao Amazawa2, Takeshi Ito1, Manabu Yasui1, Masahito Kurouchi1, Akinori Fukushima3, Takashi Tokumasu3, Seughwan Lee4, Sungkyun Park4, Hirofumi Takikawa5, and Mamoru Yoshimoto6

1Kanagawa Industrial Technology Research Institute, Ebina, Kanagawa 243-0435, Japan
2JSW AFTY Corporation, Hachiogi, Tokyo 192-0918, Japan
3Tohoku University, Sendai 980-8577, Japan
4Pusan National University, Busan 609-735, Korea
5Toyohashi University of Technology, Toyohashi, Aichi 441-8580, Japan
6Tokyo Institute of Technology, Yokohama 226-8503, Japan

Received March 31, 2014; accepted August 2, 2014; published online October 24, 2014

Wurtzite aluminum nitride is prepared on a c-plane sapphire substrate by electron cyclotron resonance plasma-enhanced sputtering deposition (ECR sputtering). Atomic force microscopy (AFM) showed flat AlN thin-film surfaces, and X-ray diffraction (XRD) analysis verified the epitaxial growth of AlN films with the full-width at half-maximum (FWHM) of the rocking curve of 0.025 deg on the film with the thickness of 100 nm. XRD analysis also verified the change in the peak position for the AlN film along both out-of-plane and in-plane directions. The effect of lattice constants on the energy gap was theoretically estimated by the first principles method. © 2014 The Japan Society of Applied Physics

1. Introduction

Wurtzite aluminum nitride (hex-AlN) is a well-known wide-bandgap semiconductor1–5 with many aspects such as a large piezoelectric property, good optical properties,6) and a high ultrasonic velocity. Optoelectronics devices, such as high-brightness light-emitting devices, are expected as applications of the wide bandgap of hex-AlN, surface acoustic wave (SAW) modulators,7) and film bulk acoustic wave (BAW) resonators. As a light-emitting device, the emission wavelength can be varied by using different nitride alloys such as indium nitride and gallium nitride as well as aluminum nitride. The emitting wavelength can be varied between infrared to vacuum violet.

Many techniques have been used to prepare AlN thin films, such as sputtering, pulsed laser deposition, and molecular beam epitaxy7–15) and strain is always induced by large differences in lattice constants and thermal expansions between the substrate and thin films, and many properties can be affected by this strain in the films.16,17) By controlling stress through the use of a buffer layer between nitrides and the oxide substrate, Rieger et al. investigated the effect of stress on the energy bandgap.18) The construction of lattice constants has been studied on MgO thin films –15) and strain is always induced by large differences in lattice constants and thermal expansions between the substrate and thin films, and many properties can be affected by this strain in the films.16,17) By controlling stress through the use of a buffer layer between nitrides and the oxide substrate, Rieger et al. investigated the effect of stress on the energy bandgap.18) The construction of lattice constants has been studied on MgO thin films.

2. Experimental procedure

AlN thin films were deposited on c-plane sapphire substrates of Al2O3(001), using a solid-source ECR plasma system (JWS-AFTY AFTEX-6000).23) The substrate temperature was maintained, using a ramp heater, from room temperature to 400 °C. The microwave (MW) and radio frequency (RF) powers were both set to be 500 W. The substrate holder with a diameter of 6 in. was placed facing the target, as shown in Fig. 1. The details of the deposition conditions are shown in Table 1. More details such as the uniformity of film thickness can be found elsewhere.24)

After film deposition, the crystal structure was examined by XRD (PANalytical X’pert MRD) using an ordinal θ–2θ, a φ scan, a pole figure as well as a rocking curve, and the surface morphology was evaluated by atomic force microscopy (AFM). Transparency was also evaluated using a spectrophotometer (JASCO V-650).

The bandgap $E_g$ was estimated using the ABINIT code,25) a common project of the Universite Catholique de Louvain, based on the density functional theory (DFT). A parallel version of ABINIT was compiled using OpenMPI [URL: www.open-mpi.org] and performed on an Apple MacPro with eight cores of Intel Xeon. The Brillouin zone integrations were performed using a $5 \times 5 \times 4$ k-point grid in all cases. The self-consistent GW calculations were

---

1. Introduction

Wurtzite aluminum nitride (hex-AlN) is a well-known wide-bandgap semiconductor with many aspects such as a large piezoelectric property, good optical properties, and a high ultrasonic velocity. Optoelectronics devices, such as high-brightness light-emitting devices, are expected as applications of the wide bandgap of hex-AlN, surface acoustic wave (SAW) modulators, and film bulk acoustic wave (BAW) resonators. As a light-emitting device, the emission wavelength can be varied by using different nitride alloys such as indium nitride and gallium nitride as well as aluminum nitride. The emitting wavelength can be varied between infrared to vacuum violet.

Many techniques have been used to prepare AlN thin films, such as sputtering, pulsed laser deposition, and molecular beam epitaxy, and strain is always induced by large differences in lattice constants and thermal expansions between the substrate and thin films, and many properties can be affected by this strain in the films. By controlling stress through the use of a buffer layer between nitrides and the oxide substrate, Rieger et al. investigated the effect of stress on the energy bandgap. The construction of lattice constants has been studied on MgO thin films.

2. Experimental procedure

AlN thin films were deposited on c-plane sapphire substrates of Al2O3(001), using a solid-source ECR plasma system. The substrate temperature was maintained, using a ramp heater, from room temperature to 400 °C. The microwave (MW) and radio frequency (RF) powers were both set to be 500 W. The substrate holder with a diameter of 6 in. was placed facing the target, as shown in Fig. 1. The details of the deposition conditions are shown in Table 1. More details such as the uniformity of film thickness can be found elsewhere.

After film deposition, the crystal structure was examined by XRD (PANalytical X’pert MRD) using an ordinal θ–2θ, a φ scan, a pole figure as well as a rocking curve, and the surface morphology was evaluated by atomic force microscopy (AFM). Transparency was also evaluated using a spectrophotometer.

The bandgap $E_g$ was estimated using the ABINIT code, a common project of the Universite Catholique de Louvain, based on the density functional theory (DFT). A parallel version of ABINIT was compiled using OpenMPI and performed on an Apple MacPro with eight cores of Intel Xeon. The Brillouin zone integrations were performed using a $5 \times 5 \times 4$ k-point grid in all cases. The self-consistent GW calculations were