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

Satoru Kaneko[1,6], Hironori Torii[2], Takao Amazawa[2], Takeshi Ito[1], Manabu Yasui[1], Masahito Kurouchi[1], Akinori Fukushima[3], Takashi Tokumasu[3], Seughwan Lee[4], Sungkyun Park[4], Hirofumi Takikawa[5], and Mamoru Yoshimoto[6]

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

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Wurzite 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.

1. Introduction

Wurtzite aluminum nitride (hex-AlN) is a well-known wide-bandgap semiconductor[1–5] 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 epitaxy,[7–15] 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 deposited on silicon substrates by both pulse laser deposition (PLD) and sputtering.[19,20] AlN prepared on a sapphire substrate also showed the construction of lattice constants in this study. The lattice constants were varied along both surface normal and in-plane directions. In order to evaluate the effect of lattice constants on the bandgap, the first principles theory was employed with the GW method. The details of the crystal structure were also examined using several methods of X-ray diffraction (XRD).[21,22]

2. Experimental procedure

AlN thin films were deposited on *c*-plane sapphire substrates of Al_2O_3(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 I. More details such as the uniformity of film thickness can be found elsewhere.[24]

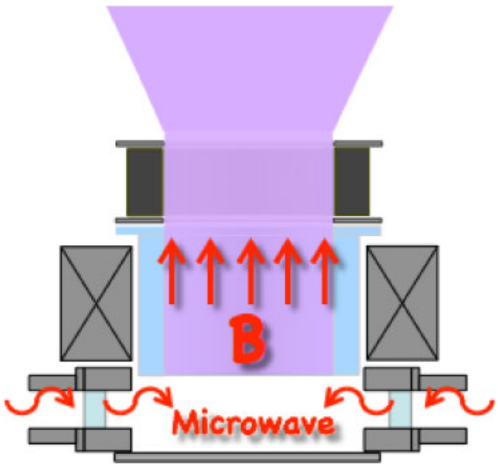

Fig. 1. (Color online) Solid-source ECR sputtering deposition system (JSW-AFTY AFTEX-6000). The substrate holder rotated during deposition and the temperature was varied using a ramp heater.

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

