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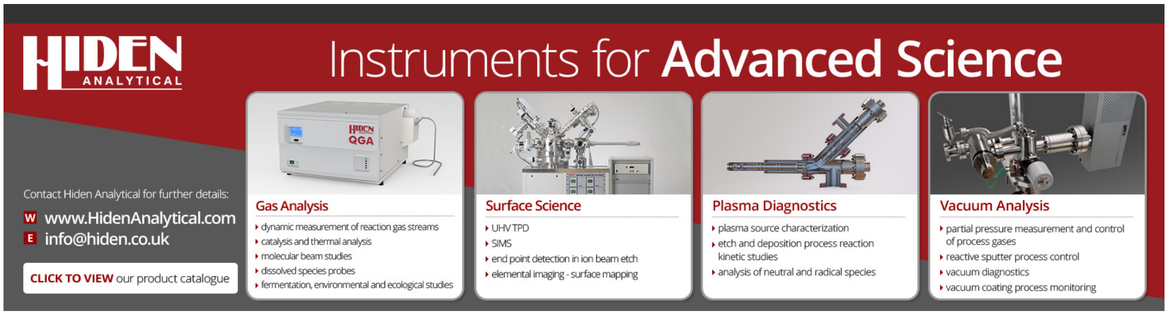

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Growth and optical characterization of aluminum nitride thin films deposited on silicon by radio-frequency sputtering

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Highly textured hexagonal aluminum nitride (AlN) thin films were deposited on silicon substrates by radio-frequency magnetron sputtering at a substrate temperature below 400 °C and annealed in the temperature range of 400–450 °C by rapid thermal annealing. The optical and the electro-optical properties have been investigated using the prism-coupling technique. Both ordinary and extraordinary refractive indices ($n_0 = 2.0058$ and $n_e = 2.0374$ at 632.8 nm) were respectively determined from the transverse electric and the transverse magnetic mode excitations. Furthermore, refractive index profiles analysis by using an improved inverse Wentzel–Kramer–Brillouin method reveals a step-like behavior of AlN thin films. The optical losses have been evaluated to be around 7 dB cm^{-1}. The electro-optic coefficient r_{13} of 0.98 pm/V has been measured from the variation of the shift of guided-modes spectrum as a function of the applied electric field in the experiment. [S0003-6951(99)03709-2]

Aluminum nitride (AlN) thin films are of increasing interest for a large number of applications in microelectronic field. Because of its wide direct band gap, AlN is a promising material for integrated optics in the ultraviolet (UV) region, i.e., laser diode,[1] detectors,[2] and fabrication of high frequency surface acoustic wave (SAW) devices.[3] Moreover, the high insulating and conducting properties of AlN can be used in the fabrication of III–V based electronic structures. Various techniques have been developed for growing thin films of AlN.[4,5] Most recent works have been performed on epitaxial growth of aluminum nitride using sapphire as a substrate.[6] However, silicon substrates offer more advantages for nitride devices over sapphire: it is ideal in integrating electronic and optical devices at low costs using established silicon technology. In this letter we report the investigation of the optical and the electro-optical properties of AlN thin films by using the prism-coupling technique.[7,8] This work is both focused on the optimization of the growth process and the comprehensive study of the relationship between the structure and the optical characteristics.

For our study, AlN films were deposited by radio-frequency (rf) magnetron sputtering on Si/SiO$_2$ substrates from aluminum nitride targets, in a gas mixture of argon (Ar) and nitrogen (N$_2$) with a purity of 99.999%, respectively. In order to improve the structural properties of nitride compounds, a two-step process was used. First, the substrate temperature was maintained at a low temperature of 400 °C in the *in situ* growth. Second, a rapid thermal annealing (RTA) process was achieved for enhancement of the crystalline quality of the material. The optimization of the growth conditions leads to a single crystal AlN with a relatively smooth surface. We found that the growth rate was about 5 nm/min. The sputtering conditions are listed in Table I.

To investigate the structural properties of our AlN thin films, we used the x-ray diffractions (XRD) patterns in the θ–2θ configuration, as reported in Fig. 1. The growth direction for AlN films is (002), the best texture is obtained at a low temperature (400 °C) with a N$_2$ content of 30%. The orientation of the film is generally controlled by its interaction with the substrate and by kinetics of the growth process. As reported by Dovidenko *et al.*,[5] this effect is probably caused by the grain-boundary separating individual grains. These planar defects are mainly generated in the closed-packed plane of AlN during the growth process.

For the optical characterizations, we have used the prism-coupling technique. We report in Figs. 2 and 3, on transverse electric (TE) and transverse magnetic (TM) guided-modes spectra, respectively. Five guided modes have been excited for each case. We notice the sharpness of the reflectivity dips indicating a good confinement of the light into the wave guide. Therefore, moderate optical losses in the AlN film can be suggested. Indeed, those later have been evaluated by using the charge coupled device (CCD) camera

TABLE I. Sputtering conditions for deposition of AlN thin films on silicon substrates.

Parameter	Condition
Target	AlN 99.999%, 3 in. ∅
Substrate	SiO$_2$/Si (100)
Target-substrate spacing	50 mm
Substrate temperature	400 °C
rf power	300 W
Gas pressure	1.2 mbar
Ar/N$_2$	70/30
Deposition rate	5 nm/min

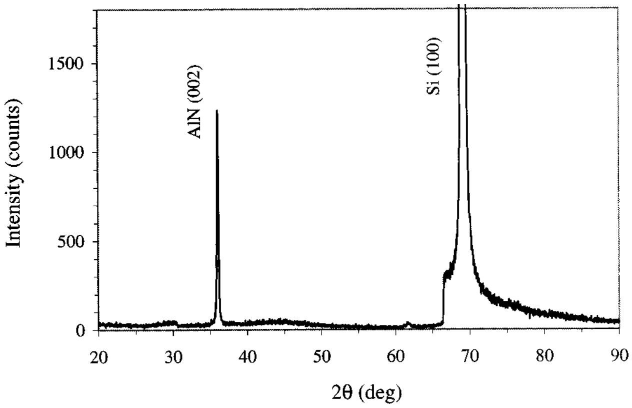


FIG. 1. X-ray diffractions patterns of aluminum nitride thin films deposited on silicon substrate.

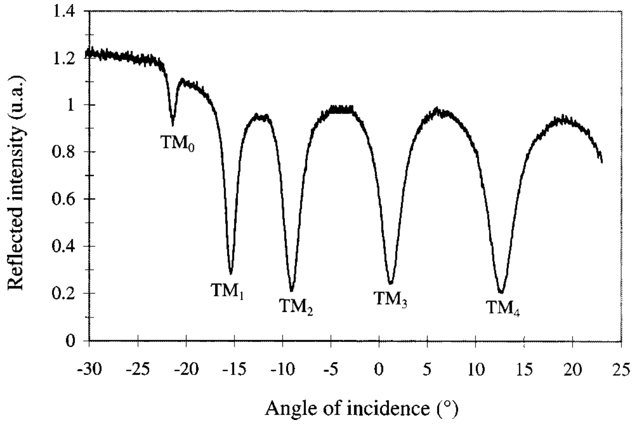


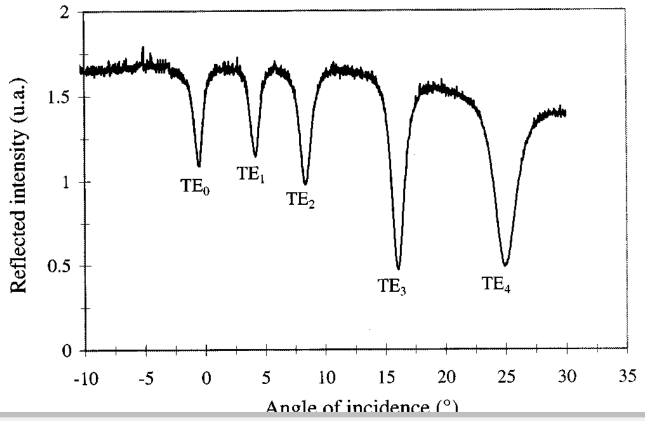
FIG. 3. TM guided mode spectra obtained by measuring the reflected intensity vs the angle of incidence (n_e excitations).

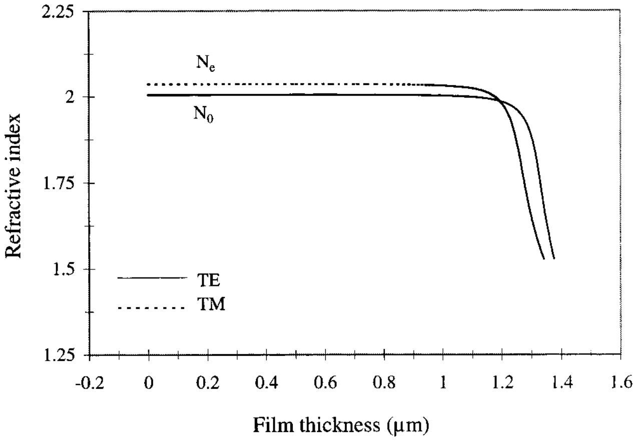
technique[9] to be in the order of 7.3 dB cm^{-1}. Higher losses have been obtained for higher-order modes excited in the film. The wave guide losses are known to be strongly dependent on the surface roughness of the film. The surface morphology of AlN samples has been examined by atomic force microscopies (AFM) showing a good surface quality for our films (r_{ms} about of 40 Å). In order to minimize the optical losses, the epitaxial growth of AlN thin films is required.

From the angular position of the guided modes, we computed the corresponding effective indices and hence the refractive indices and the film thickness. For our samples, the ordinary (n_0) and the extraordinary (n_e) refractive indices are 2.0058 ± 0.0004 and 2.0374 ± 0.0006 ($\lambda = 632.8$ nm) respectively. These values are similar to those reported in the literature.[6,10] However, slight deviations of refractive indices are obtained in comparison with the corresponding AlN single crystal ordinary refractive index n_0 which is around 2.16.[11] This is mainly attributed to the nitrogen vacancy or oxygen impurities. The thickness was determined to be $1.28 \pm 0.04\,\mu$m which is in agreement with the scanning electron microscope (SEM) investigation.

Note that in this study, we focused our attention to the simple case of light propagation in anisotropic uniaxial thin film deposited onto an isotropic substrate. In this configuration, TE and TM modes can exist separately. Therefore, the problem was treated using the well-known guided-modes dispersion equation. However, the deposition technique may yield thin films with the optical axis tilted from normal to the substrate surface. In this situation, TM modes are affected by the tilt angle (φ) of the optical axis which determines the refractive index seen by the optical wave propagating within the guiding structure. The calculation procedure[12] provides a weak tilt angle (φ) of nearly 6° with respect to the normal to the substrate surface, confirming the uniaxial nature of our AlN thin films deposited by rf sputtering, with the optical axis very likely oriented perpendicular to the substrate surface.

To complete this analysis, we have reconstructed the refractive index profiles directly from the measured effective indices by using an improved version of the inverse Wentzel–Kramer–Brillouin (*i*WKB) method. This method only depends on the refractive index distributions within the guiding layer. More details of calculation are given by Chiang.[13] Using a polynomial interpolation of the measured effective indices, we computed the refractive index profiles as a smooth function of the thickness. As shown in Fig. 4, the refractive index profiles indicate a step-index variation which is synonymous of a good optical homogeneity along the film thickness. Indeed, the refractive index remains constant within the guiding region and decreases rapidly near the film–substrate interface. Therefore, this result did not show any clear influence of the substrate on the growth process.





Using TE guided modes, we have investigated the electrooptic (EO) coefficient using the angular shift technique as described by Boudrioua *et al.*[14] The top electrode consists of a semitransparent gold film with a thickness of 10 nm. By applying a transverse electric field through the AlN layer, a change of the resonant coupling angle ($\Delta\theta$) in the guided-modes spectrum has been observed. This effect is directly correlated to the variation of the refractive index (Δn) due to the EO effect. Finally, the linear EO coefficient r_{13} obtained is evaluated to be 0.98 pm/V.

In summary, AlN thin films have been grown on Si/SiO$_2$ substrates by radio-frequency magnetron sputtering from an aluminum nitride target. The deposition parameters and annealing process were optimized for the elaboration of highly textured AlN thin films. We have investigated the optical performances of the films using the prism-coupling technique. Refractive indices were therefore determined to be $n_0=2.0058$ and $n_e=2.0374$ at 632.8 nm. From the effective guided-mode indices, the analysis of the optical anisotropy confirmed the uniaxial nature of the AlN thin film with the optical axis likely oriented normal to the surface of the substrate. The optical losses were evaluated to be around 7 dB cm^{-1}. The EO measurements using the angular shift method showed a linear electro-optic coefficient r_{13} of about 0.98 pm/V. These results demonstrate the interest of AlN thin films to be used in integrated optics applications.

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