

# Deposition of Cubic AlN Films on MgO (100) Substrates by Laser Molecular Beam Epitaxy

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**Abstract.** Cubic AlN (c-AlN) films were deposited on MgO (100) substrates by laser molecular beam epitaxy (LMBE) technique. The crystal structure and surface morphology of deposited films with various laser pulse energy and substrate temperature were investigated. The results indicate that c-AlN films exhibit the (200) preferred orientation, showing a good epitaxial relationship with the substrate. The surface roughness of c-AlN films increases when the laser pulse energy and substrate temperature increase. The film grown at laser pulse energy of 150 mJ and substrate temperature of 700 °C shows the best crystalline quality and relatively smooth surface.

## 1. Introduction

The III-V semiconductor cubic AlN (c-AlN) is becoming one of the promising optoelectronic and microelectronic materials for its excellent properties. For example, decreased phonon scattering and easier doping are expected due to its higher crystallographic symmetry [1,2]; there does not exist polarization electrical fields in the (001) growth direction [3], etc. However, high quality c-AlN film is difficult to fabricate for it is metastable. As the development of laser molecular beam epitaxy (LMBE) technique, the precise controlling and highly nonequilibrium characteristics of LMBE process are suitable to deposit metastable c-AlN films.

According to reported literatures [4,5], high oriented c-AlN films have been obtained on lattice-matched substrates. MgO has a cubic NaCl structure, and shows a small lattice-mismatch with c-AlN. Thus, c-AlN films are expected to show high quality on MgO substrates. In this work, c-AlN films were deposited on MgO (100) substrates by LMBE, and the dependences of microstructure on laser pulse energy and substrate temperature were investigated.

## 2. Experimental procedure

A LMBE system was used to deposit AlN films on MgO (100) substrates. The growth chamber was first evacuated to  $10^{-5}$  Pa, and then MgO (100) substrates were placed opposite to the AlN (99.9% purity) target with a distance of 5 cm. Subsequently, the target was irradiated by a KrF excimer laser. During the depositions, the laser pulse energy ranged from 80 to 200 mJ and the substrate temperature ranged from 650 to 750 °C for 40 min respectively. Meanwhile, N<sub>2</sub> gas (99.999% purity) was introduced into the chamber, and the pressure was maintained as  $10^{-1}$  Pa.

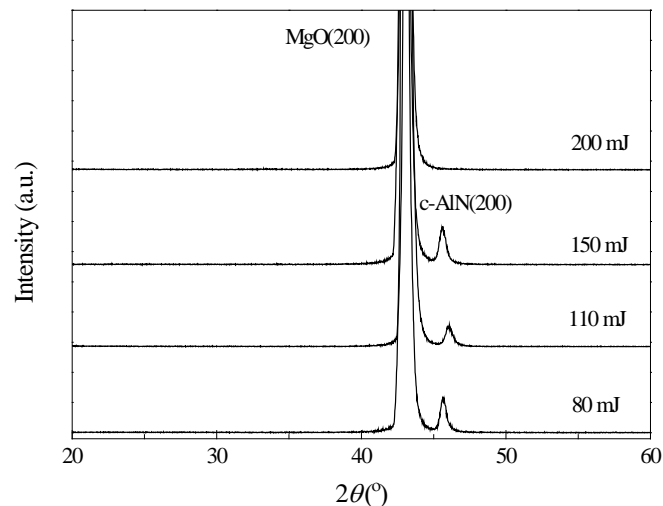


The crystal structures of films were investigated by X-ray diffraction (XRD, Rigaku D/MAX-RB) and Fourier transform infrared (FTIR) spectroscopy (Nexus 470). The surface morphologies were examined by atomic force microscopy (AFM, Agilent 5500).

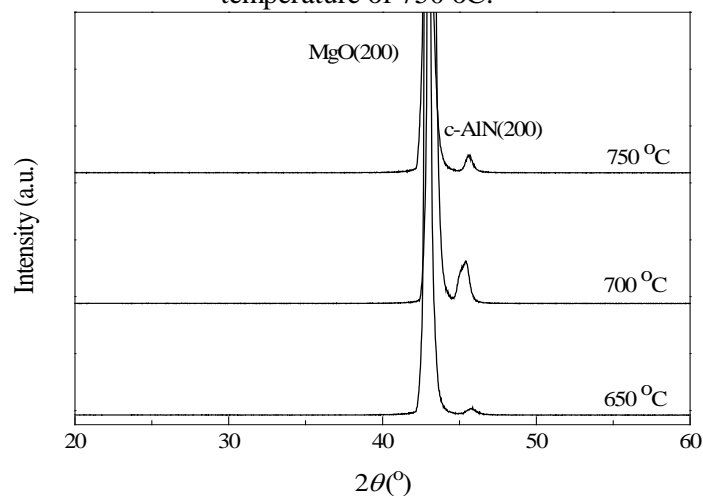
### 3. Results and discussion

#### 3.1. Crystal structure

Figure 1 displays the XRD patterns of deposited AlN films with different laser pulse energy at the substrate temperature of 750 °C. At laser pulse energies of 80, 110 and 150 mJ, deposited films exhibit a single AlN peak at around  $2\theta = 45.5^\circ$ , which is attributed to the c-AlN (200) reflex. Obviously, c-AlN films are successfully deposited on lattice-matched MgO (100) substrates. However, no AlN peaks are detected for the film deposited at 200 mJ, indicating an amorphous structure. The influence of substrate temperature on the XRD patterns of films at the laser pulse energy of 150 mJ is shown in figure 2. (200)-oriented growth is dominant for all the c-AlN films, and the intensity of (200) peak changes apparently with increasing substrate temperature. A maximum value of (200) peak is obtained at 700 °C, suggesting the good crystalline quality at this temperature.



**Figure 1.** XRD patterns of deposited AlN films as a function of laser pulse energy at the substrate temperature of 750 °C.



**Figure 2.** XRD patterns of deposited AlN films at different substrate temperature at the laser pulse energy of 150 mJ.

Based on the further analysis of XRD patterns, the grain size and lattice constant of c-AlN films are shown in table 1. The grain size changes little when the laser pulse energy increases, but the substrate temperature has more effect on it. Compared with reported results [6,7], the films in this work have a smaller grain size, indicating a good surface quality. While, the lattice constants of all films are smaller than the constant of bulk c-AlN ( $a = 0.4045$  nm), which proposes that the lattice mismatch cannot be fully released during the depositions. It can be noted that the film grown at 700 °C and 150 mJ shows the minimum grain size of 14.7 nm, and its lattice constant ( $a = 0.39888$  nm) is closest to the standard data.

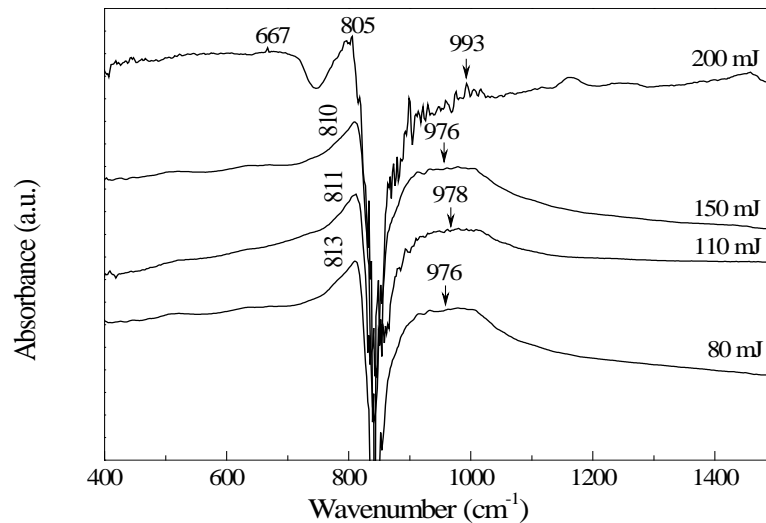
**Table 1** Grain size and lattice constant of c-AlN films with different laser pulse energy and substrate temperature.

	Laser pulse energy at 750 °C (mJ)			Substrate temperature at 150 mJ (°C)		
	80	110	150	650	700	750
Grain size (nm)	23	20.8	21.2	18.7	14.7	21.2
Lattice constant (nm)	0.39705	0.39347	0.39722	0.39547	0.39888	0.39722

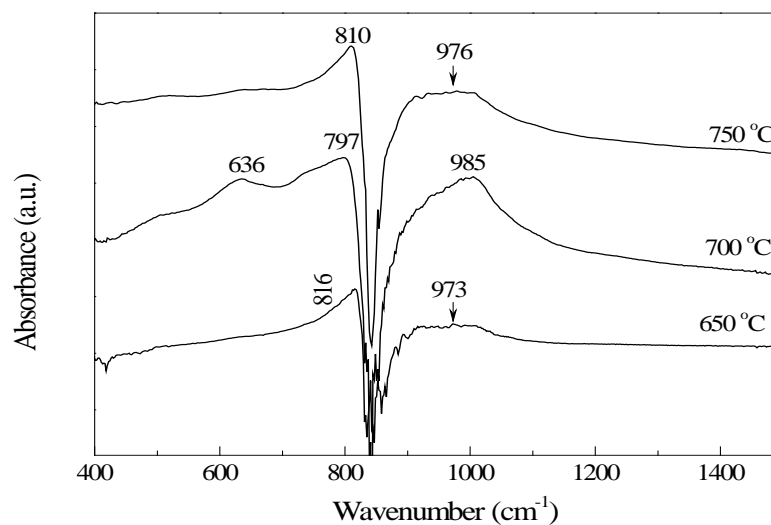
Metastable c-AlN films are difficult to deposit on Si (100) [2] or Al<sub>2</sub>O<sub>3</sub> (0001) [8] substrates for the large lattice-mismatch between them. In the present study, the lattice-matched MgO substrate acts as a template for the growth of c-AlN. And this phenomenon was also observed on the TiN (NaCl structure) buffered Si substrates [9] and 3C-SiC substrates [4]. So it is deduced that the epitaxial growth of c-AlN is significantly controlled by the crystalline plane of the substrate. As for the processing conditions investigated here, the substrate temperature plays a more important role in the crystallinity of c-AlN films compared with the laser pulse energy. In general, the mobility of atoms on the surfaces can be greatly enhanced at higher substrate temperature, which will improve the c-AlN phase formation [10].

### 3.2. FTIR analysis

Deposited AlN films are further characterized by FTIR absorbance spectra as shown in figure 3 and figure 4, in which the influence of substrates is deducted. In figure 3, two obvious absorption peaks at about 810 cm<sup>-1</sup> and 980 cm<sup>-1</sup> are observed for the films deposited with different laser pulse energy. From the reported vibration modes of c-AlN [11-12], the two peaks are assigned to the A<sub>1</sub> transverse optical (TO) and A<sub>1</sub> longitudinal optical (LO) phonon vibration modes respectively, but they both shift to the higher wavenumber. This variation may be due to the residual stress induced during the depositions, which is consistent with the XRD results. For the film deposited at 200 mJ, a weak peak at 667 cm<sup>-1</sup> is assigned to the TO phonon vibration mode of h-AlN [13], showing the poor crystalline quality of this film. The absorbance spectra of AlN films deposited at different substrate temperature show the similar absorption peaks, see figure 4. An extra peak at 636 cm<sup>-1</sup> for the film deposited at 700 °C is also detected, which corresponds to the E<sub>1</sub> TO phonon mode of c-AlN. This observation confirms the good crystalline quality of the film under this condition.



**Figure 3.** FTIR patterns of AlN films deposited at various laser pulse energy.



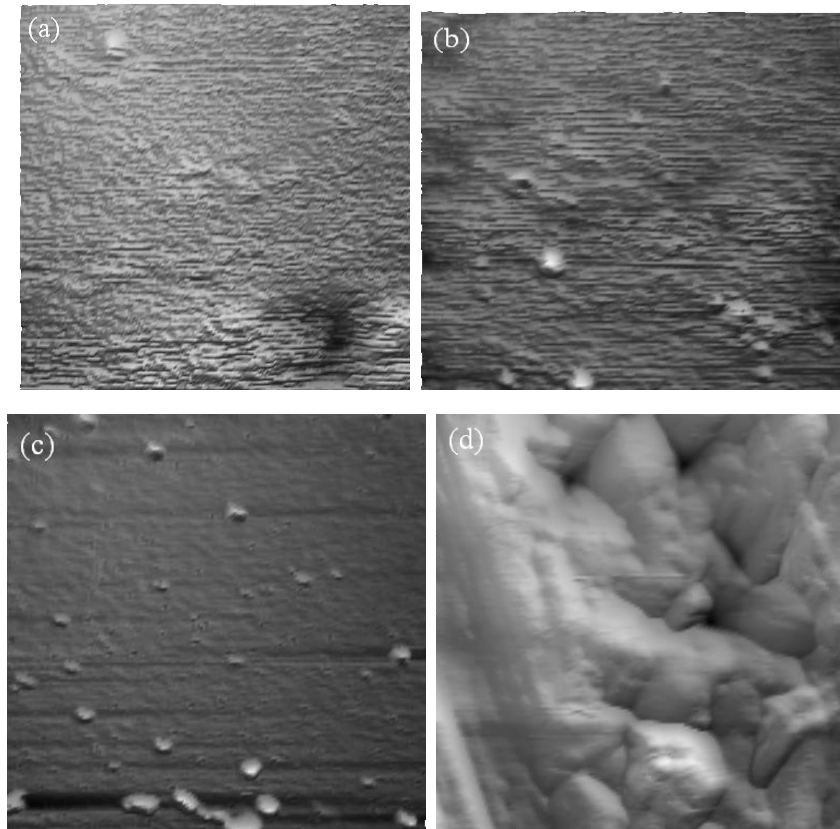
**Figure 4.** FTIR patterns of AlN films deposited at different substrate temperature.

### 3.3. Surface morphology

Figure 5 and figure 6 show the AFM surface morphologies of AlN films at different laser pulse energy and substrate temperature, respectively. It is clear that all the films are uniform, dense and relatively smooth. Both islands and terraces are observed on these surfaces owing to the Stranski-Krastanov growth mode of AlN films. The surface roughness of AlN films increases slowly when the laser pulse energy and substrate temperature are below 150 mJ and 700 °C, respectively. While a rough surface is obtained at higher laser pulse energy and substrate temperature as shown in figure 5 (d) and figure 6 (c).

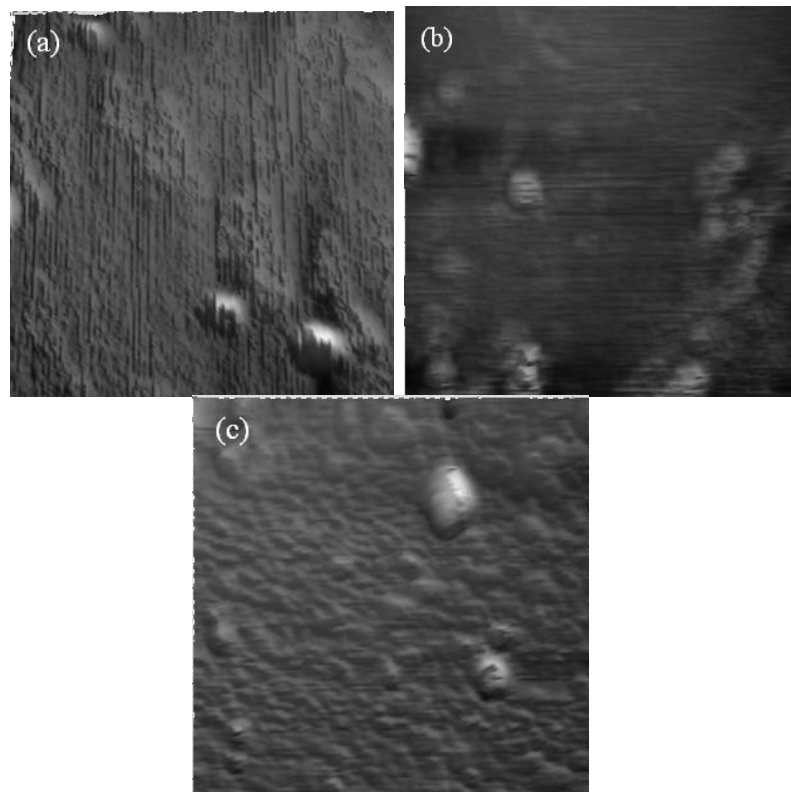
The surface roughness of AlN films deposited by LMBE technique is affected mainly by two aspects. One is the atom mobility on substrate surfaces. When the deposition rate is higher than atom mobility, the surface roughness will increase. It is known that high substrate temperature leads to high atom mobility, but atoms would be too active to settle along the low energy sites at higher temperature, resulting in large surface undulation. The other is the deposition rate on substrate surfaces. Though

higher laser pulse energy can increase the deposition rate, the sputtering damage and insufficient migration of atoms would increase the surface roughness. Thus, the proper laser pulse energy and substrate temperature for depositing c-AlN films in this study are 150 mJ and 700 °C.



**Figure 5.**  $2 \times 2 \mu\text{m}^2$  AFM surface morphology of AlN films deposited at various laser pulse energy:

(a) 80 mJ, (b) 110 mJ, (c) 150 mJ, (d) 200 mJ.



**Figure 6.**  $2 \times 2 \mu\text{m}^2$  AFM surface morphology of AlN films deposited at various substrate temperature: (a) 650 °C, (b) 700 °C, (c) 750 °C.

#### 4. Conclusions

Cubic-AlN films with high quality were grown on MgO (100) substrates using LMBE technique. (200)-oriented growth of c-AlN films is dominant, showing the orientation relationship of AlN (200) // MgO (100). The surface morphology of AlN films is featured as islands and terraces, and the surface roughness increases when the laser pulse energy and substrate temperature increases. At the laser pulse energy of 150 mJ and substrate temperature of 700 °C, c-AlN film shows the best crystalline quality and relatively smooth surface.

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