Texture growth of AlN films deposited on Si(100) and (111) by DC reactive magnetron sputtering (dcMS) and by high power impulse magnetron sputtering (HiPIMS)

A. Riah\textsuperscript{1}, A. Ayad\textsuperscript{1,2}, J. Camus\textsuperscript{3}, M.A. Djouadi\textsuperscript{3} and N. Rouag\textsuperscript{1}

\textsuperscript{1}Laboratoire Microstructures et Défauts dans les Matériaux, Université Frères Mentouri Constantine 1, Route Ain El Bey, Constantine 25017, Algeria.
\textsuperscript{2}Département de pharmacie, Faculté de Médecine, Université Constantine 3, Algeria.
\textsuperscript{3}Institut des Matériaux Jean Rouxel IMN UMR 6502, Université de Nantes, 2 rue de la Houssinière BP 32229, 44322 Nantes Cedex France.

Abstract
We have studied the texture evolution of Aluminum nitride (AlN) thin films. AlN thin films were deposited on Si (100) substrate by dc magnetron sputtering (dcMS) and High Power Impulse Magnetron Sputtering (HiPIMS) technics. We consider the influence of the deposition parameters (thickness, orientation of the substrate) on the anisotropy of the films. These films are aimed for many applications in electronics and photonics. They are used for acousto-optical filters type SAW (Surface acoustic wave) and UV emitting diodes. They are particularly useful in photonics (filter, Bragg mirror, LED, UV). Control of the anisotropy can improve the mechanical use properties of thin films. The most research works concerning AlN films have been focused on the wurtzite crystal phase, however the cubic AlN has many interesting properties, which are very different from those of the hexagonal phase. For example, is attracting more interest for its higher crystallographic symmetry, and it is expected to exhibit higher thermal conductivity, electrical resistivity, and acoustic velocity than h-AlN. Anyway this phase is still difficult to characterize.

Keywords: AlN thin films, DC-PVD, Fiber texture, Dispersion, Orientation, Asymmetry.
**Introduction**

Aluminum nitride (AlN) is a material with remarkable properties, a large optical band gap of about 5.9–6.02 eV [1], high hardness [2], chemical stability, large acoustic velocity. Moreover, AlN is fully compatible with conventional silicon technology [2,3] and has a good thermal conductivity [4]. AlN thin films are one of the most interesting materials in microelectronic and optoelectronic devices such as ultraviolet detector, light emitting diodes [5], thermal interface materials [6], dielectric layers in integrated circuits [7] and piezoelectric materials in surface acoustic wave devices [4]. The aim of this work is to investigate the effect of thickness thin and the substrate orientation on the texture evolution of AlN films deposited by dc magnetron sputtering (dcMS) and HiPIMS. Texture describes the statistical distribution of crystal grain orientations in thin films. The distribution is an important characteristic of the microstructure in thin films, and it determines various electrical, magnetic, and mechanical properties [8]

**Results and discussion**

**Part I- Texture growth of AlN on Si (100)**

1- Textures growth of AlN_H films deposited on Si (100),Si(111) substrates by dcMS:

For AlN films grown on Si (111), the fiber (0001)<u><v><w> can be considered as perfect (fig.1) with low dispersion less than 7.5° (fig.2) for plan (0001) and the texture is particularly marked. For AlN with Si (001) substrate, the fiber texture is less pronounced and more dispersed (≈ 12°) and also presents preferred orientations. The observed asymmetry increases with thickness and could be connected to the differences angular between the AlN (0001) and Si (100) which lead to full distortion.

**Figure 1.** Intensity evolution report to the azimuth angle PHI.  
**Figure 2.** Dispersion angle of (0001) fiber.

The (10-11) and (10-12) pole figure confirm the presence of reinforcements on the (0001) fiber (Fig3). The angles between these reinforcements are about 60° and 120° in the case of AlN on Si (100).

(a)  
(b)  

**Figure 3.** Experimental (10-11) (2θ= 37.89°) pole figure of AlN_H on:  
(a) AlN(2200nm)/Si(100), (b) AlN(1500nm)/Si(111)
2- Textured growth of AlN\(_H\) films deposited on Si(100) by dcMS and HiPIMS

Figure 3 and 4 shows the intensity evolution report to azimuth angle PHI, at tilt angle CHI=0, for AlN\(_H\) films deposited by dcMS and HiPIMS. For AlN\(_H\) films grown by HiPIMS, the texture is particularly marked and the fiber (0001)<\(uvw\> can be considered as perfect. Nevertheless, for AlN\(_H\) thin films deposited by dcMS, the fiber (0001) is less homogenous.

![Graphs showing intensity evolution report to azimuth angle PHI](image)

The difference of texture in the case of dcMS and HiPIMS (Figure 3 and 4) can be explained on the existence of an amorphous region with a thickness of a few nano-meters between the AlN layer and the silicon (100) substrate in the case of dcMS. Such amorphous layer may be derived from the native SiO\(_2\) layer but in the case of HiPIMS method, the interface between the film and the Si substrate is sharp, which indicates a local epitaxial growth of AlN on the Si substrate. The local absence of the amorphous SiO\(_2\) layer in the case of a deposited film by HIPIMS could be due to high ion bombardment, which likely leads to cathodic re-sputtering of the substrate and cleans the surface of the substrate at the start of film deposition. The ion bombardment may be enough to remove the SiO\(_2\) layer and thus results in a kind of continuous growth AlN preferentially oriented along c-axis on the Si substrate [9].

3- Textured growth of AlN\(_C\) films deposited on Si(100) by dcMS and HiPIMS

For AlN\(_C\), the characterization is more confused than the hexagonal phase because the peaks of AlN\(_C\) are less pronounced than those of AlN\(_H\). On the other hand, very few references exist for sake of comparison. The presence of AlN\(_C\) phase was showed on the experimental (200) pole figure for AlN\(_C\) (Figure 5) and also on (0001) AlN\(_H\) (Figure 6), which is coinciding with (111) pole figure AlN\(_C\) (2\(\theta\)= 37.78°). The high intensity of (0001) fiber hides the AlN\(_C\) response (Figure 4a), we observe (111) pole figure by removing the pole figure center (Figure 4b). Noted, the (0001) fiber for AlN\(_H\) is more marked in the case of HiPIMS compared to the dcMS, while the scales of intensity are almost identical for AlN\(_C\), in both dcMS and HiPIMS.

![Pole figures showing experimental (200) pole figure](image)

Figure 5. Experimental \{200\} pole figure (2\(\theta\)= 43.91°) of AlN\(_C\) : (a) dcMS, (b) HiPIMS.
Part II- The different possibility of growth of AlN on Si (100)

The most research works concerning AlN films have been focused on the wurtzite crystal phase. However, the cubic AlN has many interesting properties, which are very different from those of the hexagonal phase. For example, it is attracting more interest for its higher crystallographic symmetry, and it is expected to exhibit higher thermal conductivity, electrical resistivity, and acoustic velocity than h-AlN. Anyway, this phase is still difficult to characterize [10]. In other III-V compounds, cubic films of GaN and InN have been epitaxially grown on various substrates. Atomic radius and ionization energy of Al are almost the same as those of Ga. Thus, it is expected that politype of AlN films is controllable by selecting suitable growth conditions such as substrate crystal structure, substrate orientation, and lattice matching between the film and the substrate. However, there have been few reports which suggested the epitaxial growth of c-AlN on TiN and Si substrates. In this part, we report the different possibility on the growth of AlN films on Si (100). The atomic arrangements are shown in figure 7.
Figure 7. The atomic arrangements of (a) the epitaxial (100) AlN_C/(100) Si interface, (b) the epitaxial (0001) AlN_H/(100) Si interface and (c) AlN_H(0001)/AlN_C(100). ●Si, ○, N ○ Since there is probably no epitaxial relationship between AlN_H and Si (100) similar to the case between AlN_H and TiN(100) and MgO(100), there are actually two epitaxial relationship between AlN_H and (001) silicon, a type of terrace following the orientation of the silicon dimers (0001) AlN // (001) Si and [-2110] AlN1 // [01-10] AlN2 // [110] Si. The AlN epitaxial layer is composed of two fields
which are rotated 30° relative to each other. The presence of two fields generates a high density of defects and it is particularly difficult to optimize the growth parameters to get a smooth growth front [11]. The interfacial energy at AlN_C/Si (100) and AlN_H/AlN_C should be relatively small than the energy at AlN_H on Si (100). In the case of GaN, it has been demonstrated that epitaxial growth of GaN_C and GaN_H was controlled only by changing the growth conditions [12]. In our case, we hypothesize that very thin sphalerite-type AlN_C layer was formed on Si(100) by PVD methods, this thin layer favors the grown of AlN_H similar to the case of AlN on MgO (100)[13].

Conclusions
We have made a comparative study of the texture evolution of AlN films (3μm thick) deposited by conventional dcMS and HiPIMS. For AlN_H, the texture is particularly marked in the case of HiPIMS and the fiber (0001)<uviw> can be considered as perfect, with low dispersion. HiPIMS method gives a more perfect fiber with low dispersion (5°) while the dcMS gives an asymmetric fiber, with preferred orientations. Moreover, for AlN_C, our first results show its presence in all samples, suggesting that it is reoriented under stress effect and does not appear as a metastable phase, as generally admitted.

References