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Growth assessment of (002)-oriented AlN thin films on Ti bottom electrode deposited on silicon and kapton substrates

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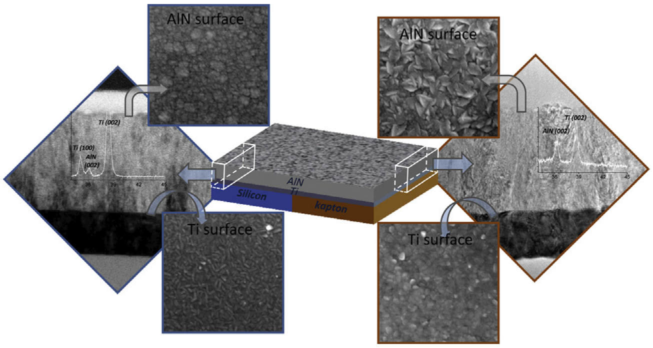
HIGHLIGHTS

- AlN/Ti system was deposited by RF sputtering on Si/SiO_2 and kapton substrates for piezoelectric application.
- Chamber pressure and RF power, were changed during Ti growth to promote (002)-orientation of the overgrown AlN layer.
- AlN(002) films were successfully obtained on Ti layers, at the highest pressure on kapton substrate and highest power on Si one.
- The achievement of AlN (002) orientation is particularly important on kapton substrate for piezoelectric flexible electronics.

GRAPHICAL ABSTRACT



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ABSTRACT

In the present work, the sputtering deposition conditions allowing the achievement of (002)-oriented aluminum nitride (AlN) thin films on titanium (Ti) bottom electrode were assessed on both silicon and kapton substrates. The AlN grain orientation was enhanced by tuning the conditions used for the Ti deposition, particularly the radiofrequency (RF) power applied to Ti target and the total pressure in the deposition chamber. Sputtered species energy and their flux towards the substrate were identified as key parameters to interpret Ti structure and morphology on both substrates, and to understand how they drive the AlN crystallization process. The evolution of morphology and structure of single Ti films and of the AlN/Ti system was characterized by X-ray Diffraction, Scanning Electron Microscopy and Transmission Electron Microscopy. Highly oriented AlN films were obtained on both substrates when the underneath Ti layer was mainly (002)-oriented; the presence in the Ti films of grains with (100) orientation produced a degree of misorientation in the following AlN growth, also resulting in a significant change of the surface morphology, on both substrates. The successful deposition of AlN/Ti on kapton substrate represents a promising result for the integration of this material in flexible piezoelectric electronics.

1. Introduction

Since piezoelectric ceramics were developed in the middle of the twentieth century, their properties have been intensively studied by a large number of researchers [1]. The possibility to convert mechanical strain energy into electrical charge (direct piezoelectric effect) or applied electrical energy into mechanical strain (inverse piezoelectric effect) has permitted to consider piezoelectric materials as a source of clean energy, when integrated in systems designed for electric power generation. The most used piezoelectric thin films are lead zirconate titanate (PZT), zinc oxide (ZnO), and aluminum nitride (AlN). PZT is

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generally employed for energy harvesting applications, thanks to its higher electromechanical coupling coefficient (k) and piezoelectric strain coefficient (d) over ZnO and AlN. On the other hand, compared to AlN and ZnO, it shows two main drawbacks: the presence of lead and the low Curie temperature [2]. The second candidate, ZnO, has better piezoelectric performances over AlN, thanks to its higher d and k values. But, unfortunately, its performances degrade at high temperature, due to its low Curie temperature compared to AlN. AlN shows great technological advantages in microelectronics industry, due to its wide bandgap (6.2 eV), high thermal conductivity (3.3 W K^{-1} cm^{-1}), and high electrical resistivity (10^{13} Ω/cm) for applications in high power electronics (HEMTs) and optoelectronics [3]. The key AlN property, which makes it more attractive than ZnO, is its lower permittivity, desirable for higher voltage generation. Moreover, AlN is not a ferroelectric material and therefore it does not require poling, like PZT. Its comparatively high piezoelectric coefficients, high acoustic velocity of 12,000 m/s, and CMOS compatibility permit a large use of AlN in RF MEMS devices. The piezoelectric property of AlN remains the same at high temperatures, thus coupling AlN and 3C-SiC for RF MEMS devices and piezoelectric actuators can be made for harsh environment applications [4].

In the specific case of piezoelectric applications, the performance of the device strongly depends on the AlN structural properties, because AlN thin films exhibit a piezoelectric behavior when they are properly oriented on a compatible substrate. In particular, AlN thin films grown along c-axis orientation (preferential growth perpendicular to the substrate) are the most interesting ones, since they exhibit properties similar to monocrystalline AlN [5] and they show intense piezoelectric response, as the (0001) orientation has the highest piezoelectric stress constant, as also reported in the latest literature [6,7,8].

Most of the devices, based on the use of piezoelectric effect, requires the fabrication of a metal layer that works as thin conductive underlying electrode on which the piezoelectric layer is deposited. Its physical properties must be compatible with the fabrication technology used for the fabrication of the device. There are many metals which, if properly oriented, are suitable as bottom electrodes for subsequent deposition of wurtzite AlN film, such as Al (111), Pt (001), Ti (001) and Mo (110) [9]. Ti electrode is ideal because of its hexagonal lattice parameters (a = 2.950 Å, c = 4.683 Å) very close to the AlN ones (a = 3.111 Å, c = 4.979 Å), thus minimizing the lattice mismatch. Moreover, Ti exhibits many advantages for microelectronics: good electric conductivity, extraordinary chemical resistivity, thermal stability, high hardness and high melting point. The control of the Ti thin film crystallographic orientation is crucial for the texture of the successive deposited piezoelectric layers, therefore the optimization of the process parameters for the metal layer deposition is crucial.

In parallel with the increasing interest towards piezoelectric material, a particular attention towards flexible piezoelectric devices is increasing too, with the exceptional opportunity for their use in bio-integrated applications. This permits, for example, to employ the mechanical energy existing in human body such as motion of the heart, contraction/relaxation of the diaphragm and lungs [10,11]: flexible electronics with recent advances in nanotechnology allow the creation of such devices. Silicon and kapton were selected as substrates due to their well assessed use in conventional and flexible microelectronics. As matter of fact, silicon is the most widely used semiconductor material for Integrated Circuits (ICs) due to the combination of physical properties and low cost as well as for its well established and documented treatments and fabrication processes; kapton is largely employed as flexible substrate in all the applications requiring polyimide films with an excellent balance of electrical, chemical and mechanical properties over a wide temperature range.

Within this frame, the aim of our work was to optimize the growth process, both on Si and kapton substrates, to obtain the proper AlN orientation in combination with a Ti bottom electrode; this is fundamental for the integration of this material in conventional and flexible piezoelectric devices, where the bilayer electrode/AlN film has to be used for the response and transduction of the piezoelectric signal.

2. Experimental details

Aluminum nitride (AlN) thin films were deposited on Ti bottom electrode by RF magnetron sputtering by using two types of substrate: 500 nm thick SiO_2 on (100) Si (Si/SiO_2) and kapton. Kapton polyimide film 100H (Dupont-Toray Inc., thickness 250 μm) was chosen as flexible substrate owing to its excellent mechanical and electrical properties, chemical stability, and wide operating temperature range (−269 °C to +400 °C). The polymeric foil was attached to a silicon wafer by silicone (Polydimethylsiloxane, PDMS Sylgard 184), which acted as a support substrate throughout the deposition process and was removed prior to testing.

AlN films, 250 nm-thick, were deposited in a RF magnetron sputtering system by using a 99.999% pure Al target, in pure Ar and N_2 gas mixture, which was introduced into the chamber by separate mass flow controllers. The base pressure of the sputtering chamber was 2×10^{-7} mbar before depositions. The N_2 flux percentage in the reactive mixture was fixed at 60%, the RF power applied to Al target at 150 W and the total pressure at 4×10^{-3} mbar. The substrates were not intentionally heated during the growth process and the temperature never exceeded 50 °C. The target-substrate distance was fixed to 80 mm. Before the deposition of the AlN layer, a 100 nm-thick Ti bottom electrode was deposited on the Si/SiO_2 and kapton substrates, by using different process pressure and RF power applied to the Ti target. The effect of the metal underlayer structure and morphology on the physical properties of AlN thin film in relation with the substrate type has been investigated.

The crystalline structure and crystal orientation of both Ti and AlN films were analyzed by X-ray diffraction by using the Cu-Kα radiation and scanning angle of $2\theta = 30°–60°$. The strain and crystallite size of the thin films were extracted from the XRD data by standard methods. Strain is calculated from $\varepsilon_z = (c - c_0) / c_0$, where c_0 is the strain-free lattice parameter (4.979 Å) and c is the experimental lattice constant

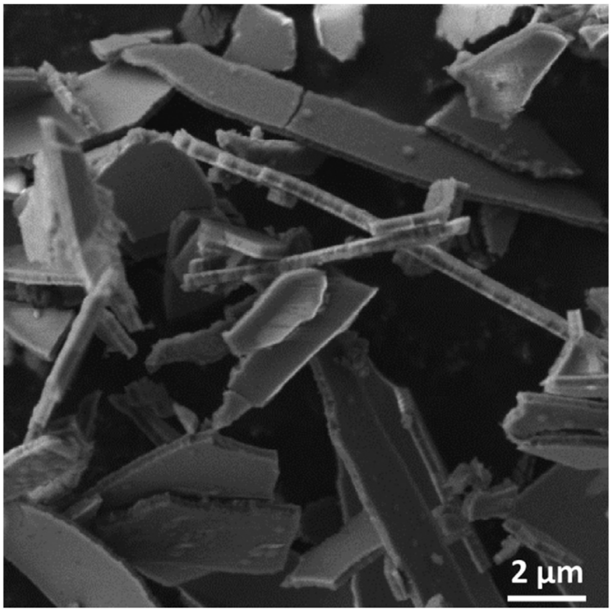

Fig. 1. SEM image of the AlN/Ti film transferred from kapton substrate to the carbon tape for cross section analysis.