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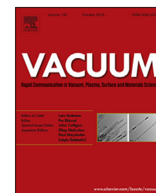

Short communication

Influence of silicon crystal orientation on piezoelectric textured aluminium nitride deposited on metal electrodes

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There is a demand for enhancing the piezoelectric properties of aluminium nitride for MEMS applications. This paper investigates the crystallinity and piezoelectric properties of AlN and how they are affected by the crystal structure of the underlying layers. Stacks of metal/AlN were deposited on silicon wafers with different crystal orientations. Three different metals were used (Ti, Al, and Pt) as the bottom electrode in order to determine if the effects are dependent on a particular metal layer. The rocking-curve FWHM of AlN was decreased by approximately 32–35% when the metal/AlN layer was deposited on (111) Si compared to (100) Si, due to the reduced atomic mismatch. The increased (002) orientation of AlN significantly affected the piezoelectric properties resulting in a (d_{33}) increase from 2.68 to 6.09 pm V^{-1} on Al, −5.01 to −6.31 pm V^{-1} on Ti, and −5.48 to −7.15 pm V^{-1} on Pt metal electrodes.

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Aluminum nitride (AlN) is a III-nitride material that has interesting properties for numerous applications, and its use in both optics and MEMS devices is continuing to grow. It is often used as a buffer material to promote growth or to create an alloy with GaN for use in optical devices [1]. However, this paper is interested in its piezoelectric properties for MEMS applications because of its compatibility with MEMS processing. AlN has been widely used in MEMS devices consisting of energy harvesters [2,3], resonators [4], sensors [5,6], and actuators [7,8].

AlN typically has lower piezoelectric properties when compared to other piezoelectric or ferroelectric materials, but its CMOS compatibility makes it an ideal material for MEMS applications. Therefore, there is an interest to enhance the piezoelectric properties in order to enhance device performance. Most of the recent research on enhancing the properties has focused on creating an alloy material by co-sputtering AlN with Sc [9,10]. However, other methods such as controlling polarity, deposition parameters, and enhancing crystallinity have also been investigated. The piezoelectric properties of AlN are dependent on the crystallinity of the textured c-axis (002) oriented AlN material. Therefore increasing the crystallinity is critical to enhancing the piezoelectric properties.

In optical applications AlN is deposited directly on the substrate. However, most piezoelectric applications require a metal interlayer between the substrate and AlN to act as a bottom electrode. There has been extensive research on improving the crystallinity of AlN by modifying the underlying metal electrode [11–13]. The crystal structures and crystallinity of the metal layers can significantly affect the quality of the AlN film. However, research on how the substrate layers crystal structure and crystallinity affects the piezoelectric properties of AlN is limited [14]. The substrate layers crystal structure and lattice mismatch properties with AlN have been investigated for optical device applications, where AlN was deposited/grown directly on the substrate (sapphire or Si) in order to promote growth of GaN. The AlN crystallinity was demonstrated to be dependent on the atomic mismatch between the substrate and AlN, when the AlN was deposited/grown directly on the substrate [1,15]. However, most MEMS applications use AlN for its piezoelectric properties, which require deposition of AlN onto a conducting electrode. The affects of the crystal orientation of the initial substrate on the metal/AlN stacks are of significant interest to MEMS applications, which has not been previously reported.

This paper aims to validate that the AlN crystallinity and piezoelectric properties can be enhanced by reducing the atomic mismatch between all underlying layers. This paper investigates the effects of depositing metal/AlN stacks onto Si substrates with different crystal orientation. The effects are demonstrated by investigating the crystallinity and piezoelectric properties of AlN. Si was used as the initial substrate as it is widely used in MEMS applications. (100) Si is the most commonly used crystal orientation for MEMS devices, because it is widely available and it can be easily etched using wet-etching techniques. However, (111) Si has an

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improved lattice match between the metal/AlN layers and the Si substrate, but it is typically requires a dry etching technique in order to pattern it. Enhancement of the piezoelectric properties is important to MEMS devices, and achieving this by changing the initial substrate material is a feasible option for most MEMS fabrication processes. In MEMS applications the Si substrate is often used for its mechanical properties, so the orientation of the Si is typically not critical.

In order to investigate the effects of Si crystal orientation on textured AlN several different crystal orientations templates were used as the initial substrate. The multi-layered structure consists of Si/metal/AlN, where the crystal orientation of the Si was varied along with the metal layer in order to validate that the effects are not dependent on the metal substrate layer. Silicon wafers with (100), (110), and (111) crystal orientation were investigated as the initial substrate material. The metal layers consisted of Ti, Al, and Pt, which were selected based on previous research and their wide-spread use as bottom electrode layers for AlN in MEMS devices [11–13,16]. These metal layers were also selected because they have varying crystal structures, consisting of hexagonal (Ti) and f.c.c (Al and Pt). AlN is a wurtzite structure, which matches well with hexagonal structures such as (002) Ti. However, a (111) textured f.c.c crystal structure demonstrates close atomic matching to c-axis aligned AlN [17]. Therefore each metal layer has a similar structure to AlN. The different crystal structures were chosen in order to investigate if the Si crystal orientation has the same affect independent of the metal electrode.

The AlN layer was deposited using reactive DC sputtering using a previously described process [18]. A 99.99% Al target was used in a 100% N_2 environment with an applied 2 kW power at 6 mT pressure with a target distance of 50 mm. The AlN deposition process remained the same for all samples. The metals were deposited onto the Si wafers using the same sputtering system, so that vacuum was maintained between depositions of the layers. The metal layers consisted of 100 nm thick metal layer followed by a 500 nm thick AlN layer. A 10 nm thick Ti layer was deposited prior to Pt in order to improve adhesion. The Si wafer was cleaned using a standard RCA clean prior to depositing metal onto the substrate. Ti/AlN was deposited onto (100), (110), and (111) Si in order to determine the effects from three different crystal lattice structures. The Al/AlN and Pt/AlN layers were deposited on (100) and (111) Si as the (111) Si has the lowest lattice mismatch between the metal and Si layers.

X-ray diffraction (XRD) measurements were used to determine the crystallinity of the layers. The measurements were performed using a (Philips X'Pert Pro 45 kV, 40 mA) [19,20]. The 2θ-ω scans were performed on the various wafers to determine the crystal structures of the material and to determine the d-spacing and lattice parameters used to calculate the atomic mismatch between layers. The inter-planar spacing (d) is found using Bragg's Law $\lambda = 2d_{hkl}\sin\theta$. The lattice parameters can be determined by using the formulas for different crystal structures.

$$Cubic: \frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \tag{1}$$

$$Hexagonal: \frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2} \tag{2}$$

Using the geometry of the hexagonal shape the c-parameter can be written as a function of the lattice parameter, so (2) can be simplified in terms of *hkl* and d-spacing as shown in (3)

$$c^2 = \frac{8}{3}a^2 \tag{3}$$

$$a^2 = \frac{4d^2}{3}\left(h^2 + hk + k^2\right) + \frac{3l^2d^2}{8} \tag{4}$$

The full-width-half-maximum (FWHM) value of the rocking curve (ω-scans) for AlN and the metal layers was used to determine the quality of the various films. The residual stresses of the layers were determined by performing a ψ-scan where the inter-planar spacing was plotted as a function of $\sin^2\psi$. The stress can be calculated using the following equation [21]:

$$\sigma = \frac{E}{1+\nu}m \tag{5}$$

where E is the elastic modulus and ν is the Poisson ratio and m is the gradient of d vs. $\sin^2\psi$. The elastic modulus of the AlN film was previously demonstrated to be 296 GPa [22]. The piezoelectric properties were determined using a piezometer (PM 300, Piezotest), which uses a standard Berlincourt method. N = 3 wafers of each type were analyzed for all experiments.

The crystallinity of the various layered structures was investigated using XRD and the results are shown in Fig. 1. The results demonstrate that the textured AlN layers consisted entirely of (002) c-axis oriented AlN in all of the samples. The Ti/AlN wafers show the peak of the various Si wafers as well as the (002) AlN and Ti peaks. The Al/AlN samples demonstrate a (002) AlN layer along with a (111) Al layer. The intensity of the AlN peak is comparable in all the samples. The 2θ-ω scans demonstrate that highly textured AlN was deposited onto each sample. The peak locations of the 2θ-ω scans were used to calculate the inter-planar spacing values, which were used to determine the atomic mismatch of the layers by calculating the lattice parameters. The atomic mismatch is calculated using the following equation [15]:

$$\varepsilon = \frac{a_S - a_f}{a_S} \tag{6}$$

where a_S and a_f are the lattice parameters of the interfacing layers. The results of the atomic mismatch are shown in Table 1. The measured lattice parameters were within 2% error of the tabulated values. The results demonstrate that (100) Si has a significantly higher mismatch to all three metal layers with values of 46.7%, 34.5%, and 38.3% for Ti, Al, and Pt respectively, whereas (110) Si had a lower mismatch with Ti of 24.6%. The atomic mismatch between (111) Si and the various metals was significantly reduced compared to the mismatch of (100) Si, with values of 7.6%, 28.8%, and 25.3% for Ti, Al, and Pt. The mismatch is considered to be high when compared to the mismatch between AlN and sapphire. However, reducing the atomic mismatch between layers should result in a higher quality material with reduced stress, which will increase the piezoelectric properties. The atomic mismatch between the metals and the AlN are significantly lower compared to metal on Si. However, an ideal layered structure would have low atomic mismatch between all of the materials.

The rocking curve FWHM value for the AlN film is typically used to determine the quality of the film and has been shown to have a significant effect on the device performance [23]. The results of the rocking curve FWHM values for AlN are visually shown in Fig. 2. All samples demonstrated a significant decrease in FWHM for materials deposited on an initial substrate of (111) Si compared to (100) Si as shown in Figs. 2 and 4a. The Ti/AlN samples demonstrated that films deposited on (110) Si had a FWHM reduction from 2.42° to 1.96°, and deposition on (111) Si further reduced the FWHM value

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