Thermal Assisted Intermixing at AlScN/Pt Interfaces

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***Abstract*—Ti/Pt/$Al_{0.6}Sc_{0.4}N$/Pt capacitor structure was fabricated. Post-annealing was carried out in nitrogen atmosphere at temperature up to 800 °C to evaluate the thermal stability of the AlScN/Pt interfaces. Material characterization revealed that the AlScN (0002) and the Pt (111) textures remained stable until the annealing temperature did not exceed 500 °C. Annealing at 600 °C and above resulted in notable Pt diffused into the AlScN film, and the bottom Pt reacted with the Si substrate to form PtSi. The thermal assisted intermixing reduced the effective dielectric thickness. Lower dielectric breakdown voltage was thus recorded.**

Keywords—scandium aluminum nitride, Pt electrode, thermal annealing, interfacial diffusion, dielectric breakdown

I. INTRODUCTION

Scandium doped aluminum nitride ($Al_{1-x}Sc_xN$, AlScN) thin films exhibit enhanced piezoelectric response and ferroelectric switching performances. The non-centrosymmetric wurtzite structure remains well in the Sc content range of $x = 0 - 0.43$. Increasing the Sc doping concentration leads to larger piezoelectric constants [1] and the easier reversion of the polarity [2]. Owing to the high thermal stability, AlScN-based devices have been identified as good candidate to work at harsh environment.

Magnetron sputtering is the most adopted technology to deposit AlScN films. In line with the electronic device design, sputter deposition of the AlScN films on metal surfaces are widely investigated. Many metal electrodes have been selected to build up AlScN-based devices. In term of AlScN (0002) texture evolution, platinum (Pt) is one of the best metals for high quality AlScN growth. Under the same sputtering conditions, the AlScN films deposited on Pt underlayer substantially showed better *c*-axis texture [5] and less misaligned grains [6]. This enhancement effect has been attributed to better lattice matching between Pt (111) and AlScN (0002) planes. In addition, thermal and chemical robustness of Pt also protects its surface from reactive contamination before AlScN film deposition.

Thermal annealing at up to 1000 °C would not induce any distinguish change of the wurtzite structure of the AlScN films [3, 4]. To ensure the reliability of the electronic device containing metal/AlScN/metal structure, robustness of the AlScN/metal interface plays equally important role. K. Bespalova et al. [7], has evaluated the AlScN crystalline structures with different top metals including molybdenum (Mo), aluminum (Al), and aluminum silicide (AlSi). The structure with Mo electrode showed stable when annealing at 1000 °C for 100 hours, while the structures with Al or AlSi electrode exhibited remarkable increase in surface roughness after annealing at 450 °C. At elevated temperature, Pt could react with its neighbor material to form PtTi [8], or PtSi [9]. Higher temperature and longer annealing duration promote the alloying processes, indicating that the alloy formation is thermal assisted reactions. Temperature-driven Pt diffusion into various III-V materials has been reported before [10]. Direct observation of intermixing at AlN/Pt interface under Transmission Electron Microscope (TEM) has been published on AlN/Pt superlattice structure after high temperature annealing [11].

In this paper, we fabricated the Ti/Pt/AlScN/Pt structures and conducted post-fabrication annealing up to 800 °C to evaluate the thermal stability of this structure. Chemical composition and microstructure were characterized to understand the thermal assisted diffusion and reaction. Electrical testing was also carried out to study the impact of thermal annealing on the electrical performance. Our findings would contribute to the AlScN-based device design and integration optimization, especially for harsh environment applications.

II. EXPERIMENTAL

A. *AlScN film deposition and Pt/AlScN/Pt test structure fabrication*

Pulsed DC magnetron reactive co-sputtering was employed to grow AlScN film on a 200 mm Ti / Pt coated Si substrate. High purity Al and Sc targets were equipped in the sputtering chamber and reactive nitrogen gas was introduced to produce nitride thin film. The DC powers applied on Al and Sc targets were individually controlled as 1000 and 774 kW, respectively. $Al_{0.6}Sc_{0.4}N$ film was obtained with a thickness of 50 nm.

The AlScN film was patterned using ion beam etching, followed by evaporation of 100 nm thick Pt film on top of the AlScN. The top Pt electrode was defined to be round pads with 100 µm in diameter.

B. *Post-annealing*

The as-fabricated Ti/Pt/AlScN/Pt structures were placed in a high vacuum furnace for thermal annealing treatment. The furnace was heated up to 300, 500, 600, and 800 °C, respectively. After 5 minutes annealing with N_2 gas flow, the chamber was cooled down in vacuum to the room temperature.

C. *Characterization*

The Ti/Pt/AlScN/Pt multi-layered film stack profile and the elemental oxidation states were characterized using an X-ray Photoelectron Spectroscopy (XPS) depth profile and core-level spectra scans. The crystal structures of wurtzite AlScN and face-centered cubic Pt were investigated using a high-resolution X-ray Diffraction (XRD) machine. Direct Current (DC) current-voltage (I-V) curves were measured using a Keithley 4200-SCS semiconductor parameter analyzer.

III. RESULTS AND DISCUSSION

XPS depth profiling provides high special resolution to characterize the elemental distribution within the Ti/Pt/AlScN/Pt multi-layered structure. Core-level spectra of N1s, Al 2s, Sc 2p, and Pt $4d_{5/2}$ were measured to determine the chemical composition. A few nm of film was then removed from sample surface by a low power Ar^+ gun. The core-level spectra were measured again. Step-by-step, the elemental concentration against film depth was obtained, as shown in Fig. 1. The 3-layered bottom Pt/AlScN/top Pt film structure of the as-fabricated sample was clearly presented in Fig. 1(a). For those annealed samples, the interfaces between Pt and AlScN became thicker, suggesting intermixing happened. As the Pt profiles shown in Fig. 1(d), more Pt diffused into AlScN as the annealing temperature increased, demonstrating that it is a thermal assisted process.

Fig. 2 displays the Pt $4d_{5/2}$, Sc 2p, N 1s, and Al 2s core level spectra recorded in middle of the AlScN films. Pt signal was not detected in the as-fabricated and the 500 °C annealed samples, while significant Pt signals were recorded in the samples annealed at 600 and 800 °C, respectively. The Pt $4d_{5/2}$ peak location at about 315 eV suggested its oxidation state is Pt^0. In addition, no peak location shift was noted on the Al 2s, Sc 2p, and N 1s core level spectra, indicating that the Pt diffused into the AlScN at ≥ 600 °C, but did not form any chemical bonds.

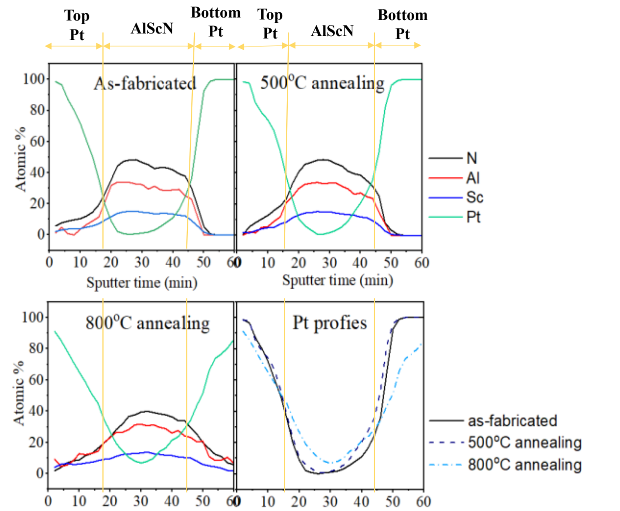

Fig. 1. XPS depth profiles of Ti/Pt/ScAlN/Pt structures. Elemental intermixing at AlScN/Pt interfaces was observed on those samples after high temperature annealing.

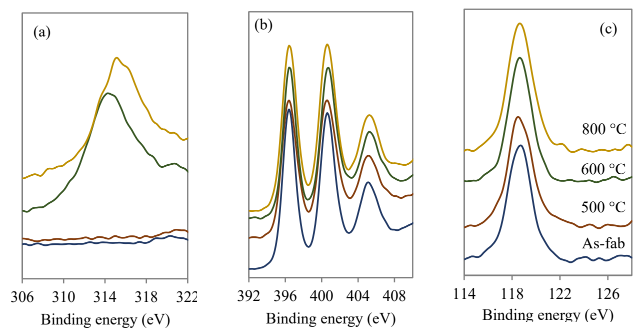

Fig. 2. XPS core level spectra of (a) Pt $4d_{5/2}$, (b) Sc 2p, N 1s, and (c) Al 2s recorded in middle of the AlScN films. Pt diffused into AlScN when the annealing temperature reached 600 °C and higher.

Fig. 3 shows high resolution XRD ω - 2θ patterns of the Ti/Pt/AlScN/Pt structures. The as-fabricated AlScN and Pt films were highly (0002) and (111) textured. These crystalline structures were well maintained when the annealing temperature did not excess 500 °C. Annealing at 600 °C and above resulted in the presence of foreign reflections peaks, which well matched with PtSi reflection pattern [12]. As pointed out in earlier studies, quick Ti and Pt interdiffusion happened at 600 °C [10], and Pt reacted with Si at 400 - 600 °C to form PtSi [12]. Annealing at ≥ 600 °C facilitated reaction between the bottom Pt electrode and the Si substrate to produce PtSi.

Fig. 4 illustrate the XRD reflection peaks evolution during the thermal annealing. Annealing at 300 – 500 °C increased the Pt (111) peak intensity and shifted the peak location towards larger 2θ direction, which correlated well to the Pt grain coarsening and stress release in the Pt lattice. No change in the AlScN (0002) peak intensity and location was noted when the annealing temperature ≤ 500 °C. Higher temperature (≥ 600 °C) annealing resulted in significant decrease in both Pt (111) and AlScN (0002) peak intensities. PtSi formation and Pt diffused into AlScN film should be responsible for these observations.

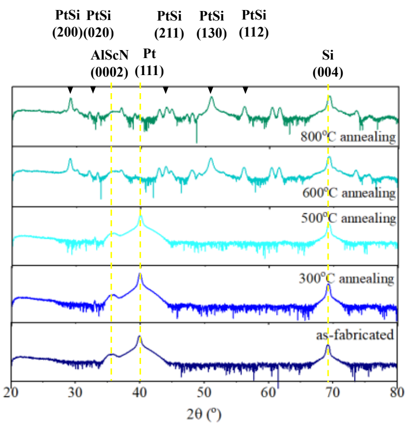

Fig. 3 XRD ω - 2θ patterns of Ti/Pt/AlScN/Pt structures. PtSi was formed in the samples annealed at ≥ 600 °C.

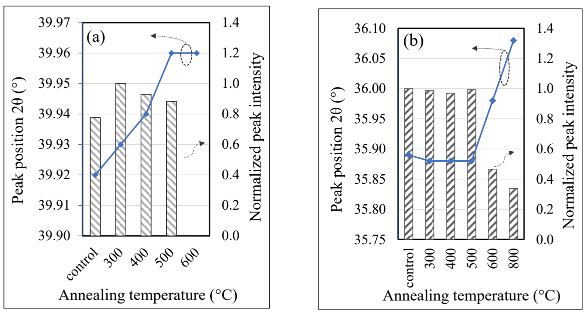

Fig. 4 Peak position and normalized peak intensities of (a) Pt (111) and (b) AlScN (0002).

DC I-V curves shown in Fig. 5 was used to evaluate the influence of annealing thermal assisted intermixing on the electrical response. Annealing at lower temperature slightly reduced the current leakage compared to the as-fabricated sample. On the 800 °C annealed sample, dielectric breakdown was recorded at lower voltage, which should be attributed to the effective dielectric thickness reduction. Thermal assisted intermixing and Pt diffusion into AlScN film would be responsible for this observation.

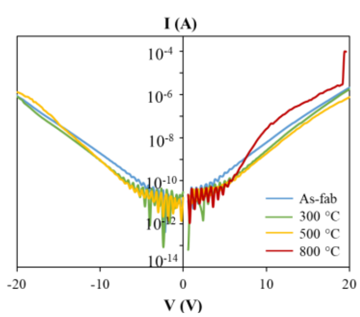

Fig. 5 DC I-V curves of Pt/AlScN/Pt structures. The thermal assisted intermixing at AlScN/Pt interfaces and Pt diffusion reduced the effective dielectric thickness and led to breakdown at lower voltage.

IV. CONCLUSIONS

Ti/Pt/$Al_{0.6}Sc_{0.4}N$/Pt test structures were fabricated, and their thermal stability were evaluated. When the annealing temperature ≤ 500 °C, AlScN (0002) and Pt (111) textures remained stable. Insignificant intermixing was found at AlScN/Pt interfaces. When the annealing temperature reached 600 °C and above, obvious elemental intermixing was found between the AlScN and Pt films. The effective dielectric thickness was thus reduced, evidenced by the lower breakdown voltage. Moreover, the bottom Pt was found to react with the Si substrate to form PtSi. Our results demonstrated that the thermal assisted intermixing impact composition, crystalline structure, and electrical properties of the metal-AlScN-metal capacitor structure. Thermal stability should be taken into well consideration during AlScN-based device design and fabrication.

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