Supplemental materials to Submission # 8147: "High Quality TiN Plasma Enhanced Atomic Layer Deposition on SiO2 Substrate with AlN Interfacial Layer via in situ Atomic Layer Annealing"

References:

[1] I. Krylov, X. Xu, Y. Qi, K. Weinfeld, V. Korchnoy, M. Eizenberg, and D. Ritter, J. Vac. Sci. Technol. A 37, 060905 (2019)

[2] Huan-Yu Shih, Wei-Hao Lee, Wei-Chung Kao, Yung-Chuan Chuang, Ray-Ming Lin, Hsin-Chih Lin, Makoto Shiojiri, and Miin-Jang Chen, Scientific Reports Volume 7, Article no: 39717 (2017)

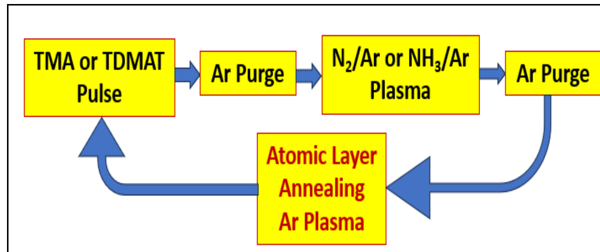


FIG. 1. The schematic diagram of the processing cycle, including the atomic layer annealing (ALA) for AlN (TMA pulse) or TiN (TDMAT pulse) on SiO_2 substrate. The ALA treatment is introduced by the in-situ Ar plasma treatment to facilitate adatom migration for improving the crystalline quality of the AlN and TiN layers

Table 1. Properties of PEALD layers deposited on SiO_2 (Si1 and Si2 samples) and on sapphire (Sa1 and Sa2 samples) with in-situ ALA

Sample	Layers	Layer thickness measured in TEM, nm	Layer thickness measured by XRR, nm	Layer density measured by XRR, g/cm^3	TiN resistivity as grown, µΩ.cm	TiN resistivity postdeposition annealing, µΩ.cm
Si1 (PEALD with N_2 plasma)	AlN	7.5	8.8	3.28	84	84
	TiN	14.5	14.6	5.26		
Si2 (PEALD with NH_3 plasma)	AlN	8	8.3	3.15	75	76
	TiN	13.8	14	5.14		
Sa1 (PEALD with N2 plasma)	AlN	6.6	7.5	3.32	10.5	10.4
	TiN	14.5	14.3	5.2		
Sa2 (PEALD with NH_3 plasma)	AlN	8.5	8.33	3.25	48	47
	TiN	14	15.6	5.3		

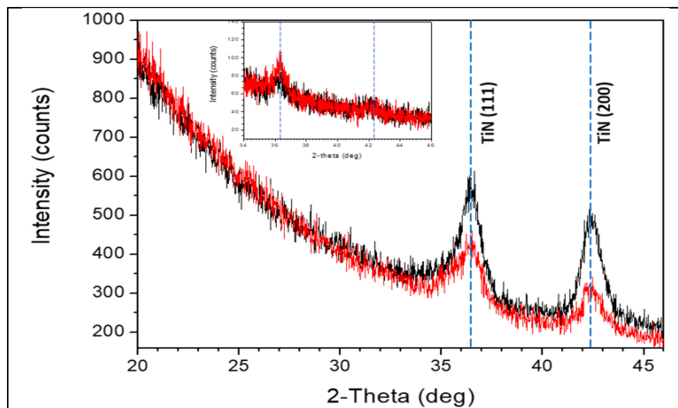


FIG. 2. XRD spectra measured using grazing angle XRD technique (ω =0.8°) for the TiN/AlN films grown on the amorphous substrate (SiO_2) with N_2 plasma (black line) and with NH_3 plasma (red line) The AlN film thickness is ~ 8 nm; the TiN film thickness is ~ 14 nm Insertion shows XRD spectra measured using θ/2θ technique for the same samples

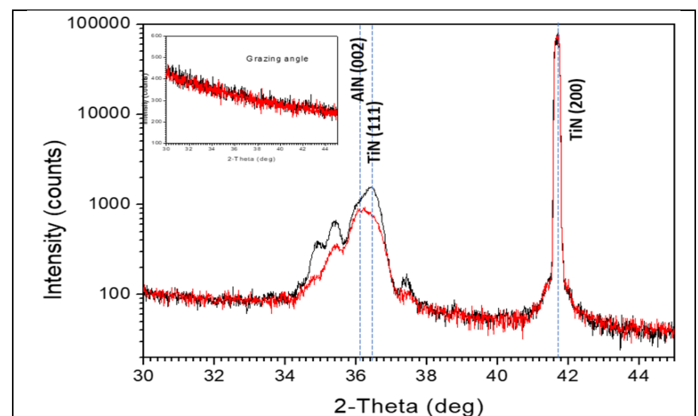


FIG. 3. XRD spectra measured using θ/2θ technique for the TiN/AlN films grown on the sapphire substrate with N_2 plasma (black line) and with NH_3 plasma (red line) The AlN film thickness is ~ 8 nm; the TiN film thickness is ~ 14 nm Insertion shows XRD spectra measured using grazing angle technique (ω = 0.8°) for the same samples

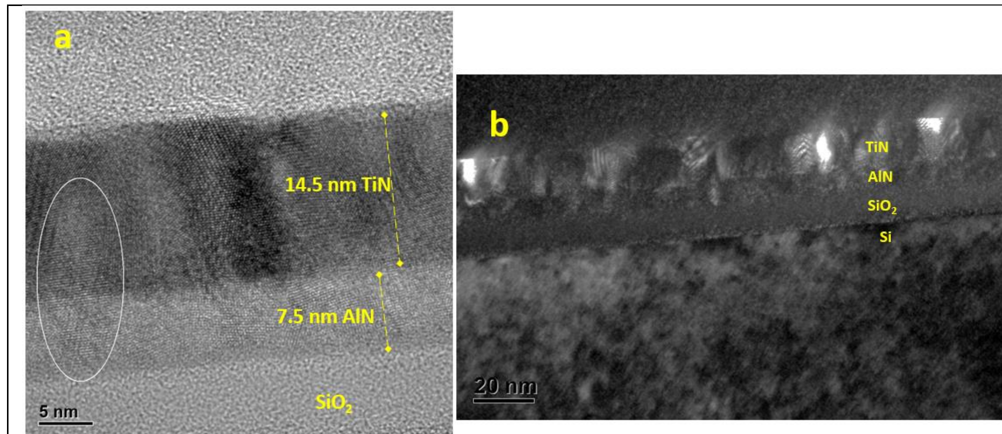
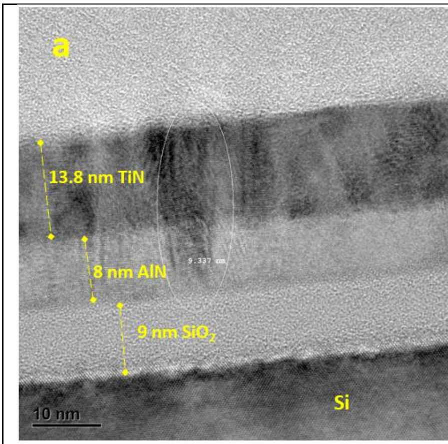


FIG.4. Micrographs of the TiN/AlN films grown on SiO_2 substrate with N_2 plasma

(a) **BF TEM lattice image**: AlN grain size in the range of ~ 2.5 - 5 nm; atomic planes of the same d-spacing which is parallel in AlN and TiN are encircled; TiN grain size is in the range of 7 - 14 nm

(b) **DF TEM**: AlN grains are randomly oriented; TiN is slightly textured



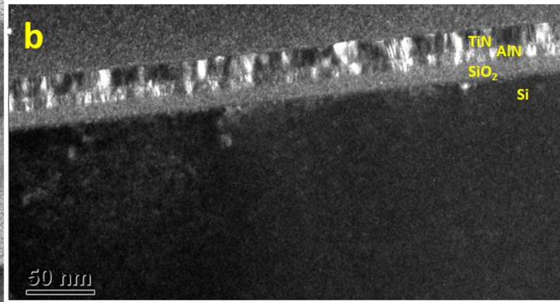
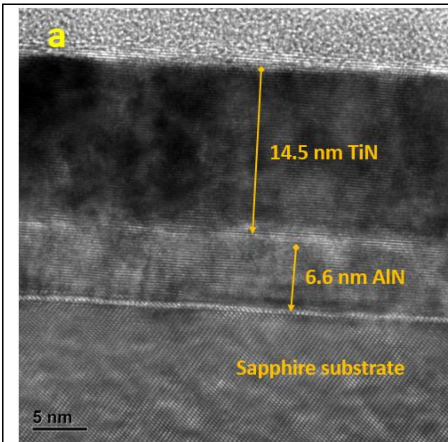


FIG.5. Micrographs of the TiN/AlN films grown on SiO_2 substrate with NH_3 plasma

(a) **BF TEM lattice image**: grain size in the range of ~ 5-9 nm; identically oriented (ca. epitaxially grown) AlN and TiN are encircled; TiN grain size about~ 6.5 -14 nm

(b) **DF TEM**: AlN and TiN are textured



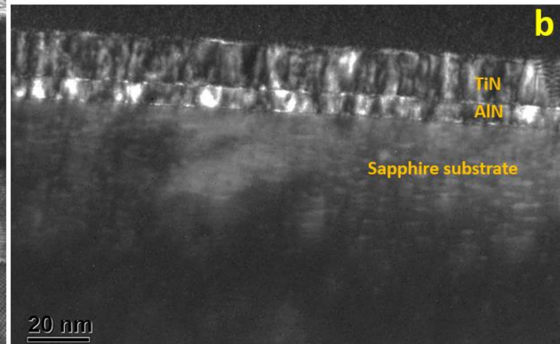
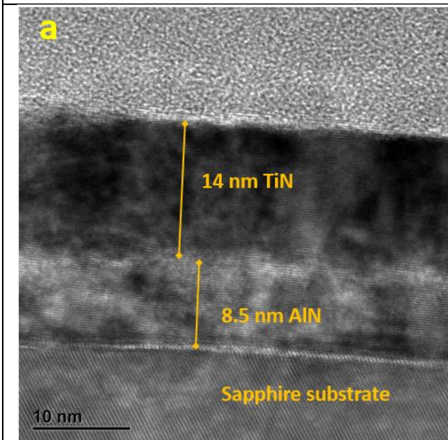


FIG.6. Micrographs of the TiN/AlN films grown on sapphire substrate with N_2 plasma

(a) **BF TEM lattice image**: AlN and TiN are perfectly in-plane textured

(b) **DF TEM:** TiN crystal size is equal to the layer thickness (~10-15 nm); presence of slightly rotated domains in AlN and TiN layers



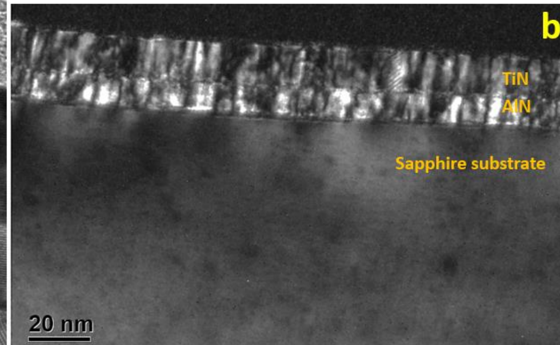


FIG.7. Micrographs of the TiN/AlN films grown on sapphire substrate with NH_3 plasma

(a) BF TEM lattice image: AlN and TiN are perfectly in-plane textured

(b) DF TEM: Crystal size is equal to the layer thickness; presence of slightly rotated domains in AlN and TiN layers