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Effect of film thickness on the properties of ultrathin tantalum nitride films

T. Srikanth[1,2], R. Subba Reddy[1], T. Vasudha[1], K. Umamaheswari[1], E. Yanadaiah[1], P. Siva[1], A. Sivasankar Reddy[1]*, V. Raja[2], P. Sreedhara Reddy[3]
[1]Department of Physics, Vikrama Simhapuri University Postgraduate Centre, Kavali -524 201, A.P., India
[2]NBKR Science & Arts College, Vidyanagar-524 411, Andhra Pradesh, India
[3]Department of Physics, Sri Venkateswara University, Tirupati- 517 502, Andhra Pradesh, India
*Corresponding Author : A. Sivasankar Reddy

ABSTRACT: *Ultrathin tantalum nitride (TaN_x) filmswere deposited on glass substrates by dc reactive magnetron sputtering at different thicknesses andanalyzed the structure,compositional, microstructure, surface morphology, optical and electrical properties. X-ray diffraction results showed that the deposited films have amorphous structure. The surface morphologies of the films were significantly affected by the films thickness. The RMS roughness of the films increased from 0.5 to 1.3nm by increasing the filmsthickness.The transmittance of the films decreased with increasing the films thickness.*
KEYWORDS: *Tantalum Nitride; Ultrathin films; Sputtering; Film thickness*

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I. INTRODUCTION

Tantalum nitride (TaN_x) is a promising material for many applications like microelectronic devices, diffusion barrier, optical coatings and thin film resistor due to their excellent properties such as high chemical and thermal stability, high wear resistance, and histocompatibility [1-5]. The properties of TaN_x thin films are extremely sensitive to the films microstructure and morphology, andare strongly depends on the deposition technique and deposition parameters[6]. TaN_x films were prepared by different thin films techniques like sputtering [7-9], cathodic arc deposition [10] and atomic layer deposition [11]. Among these techniques, sputtering is one of best techniques to prepare stoichiometry films with uniform thickness and good adhesion to substrates. In the present work, ultrathin TaN_x films were deposited on glass substrates with different thickness by dc magnetron sputtering technique and investigated their structural, compositional, microstructural, surface morphology, optical and electrical properties.

II. EXPERIMENTAL

Ultrathin TaN_x films were deposited on well cleaned glass substrates using dc magnetron sputtering. Prior to the deposition, the process chamber was evacuated until the base pressure reached under 7.8×10^{-4}Pa. The target was metallic tantalum(Ta) with purity of 99.99%. The pure nitrogen and argon were used as reactive and sputtering gases, respectively.The flow rate of argon and nitrogen were controlled by mass flow controllers. Before deposition of each film the Ta target was pre-sputtered in pure argon atmosphere for 20min in order to remove oxide layers formed if any on the target. A shutter was incorporated below the sputtering target to isolate the substrate during the pre-sputtering process. This is essential in the reactive sputtering to obtain the stoichiometry films with reproducible properties. Ultrathin TaN_x films were deposited on glass substrate with different thickness(5, 15 and 30nm) by varying the deposition time and keeping the other deposition parameters such as nitrogen partial pressures ($4x10^{-2}$Pa), substrate temperature(303K), sputtering power(100W) and sputtering pressure (2Pa) as constant. During the films deposition, the substrate holder was rotated at 15rpm to obtain homogeneous film thickness. The structural properties were characterized using X-ray diffraction (XRD). X-ray photoelectron spectroscopy (XPS) was used to determine the chemical states of the films. The microstructures and surface morphology were analyzed by field emission scanning electron microscope (FE-SEM) and atomic force microscope (AFM), respectively. The transmittance of the films was recorded by UV-Vis-NIR spectrometer. The films thickness was measured by Ellipsometer measurements. Target to substrate distance was about 80mm.

III. RESULTS AND DISCUSSIONS

Fig.1. shows the X-ray diffraction patterns of ultrathin TaN_x films at different thicknesses.The deposited films exhibited amorphous structure irrespective of the films thickness. It implies that the films deposited on amorphous substrates at room temperature with ultra-thickness is difficult to obtain a crystallinity or the samples with nano-sized thin films show lower X-ray diffraction intensity due to the noise in the recorded spectra and crystal growth orientation.Chiang et al. [12] observed that the atomic layer deposited ultrathin ZnO films with thickness of 10nm on the polished Si substrates at growth temperature of 25 and 50 ^{o}C exhibited amorphous structure.

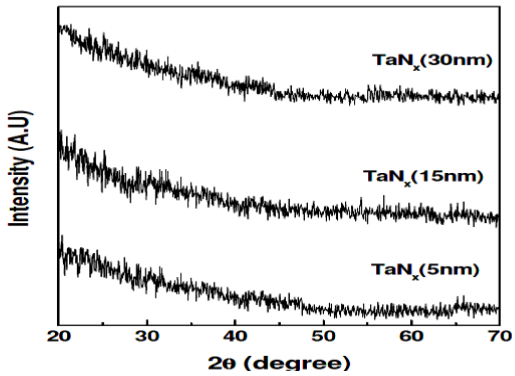

Fig.1. XRD patterns ultrathin TaN_x films at different thicknesses.

The XPS spectra of TaN_x films at different films thicknesses are shown Fig.2. From the XPS results, Ta-Ta peaks shifted to lower BE levels by increasing films thickness. The binding energy values of Ta4f in TaN_x films were 25.17eV, 27.28eV; and 24.98eV, 27.09eV for films thickness of 15 and 30nm, respectively. The present obtained binding energy values of TaN_x films at different thicknessesare not coincide with Ta (Ta4f=21.9eV), TaN_x (22.2eV, 24.1eV) and TaO_x (26.4eV, 28.3eV) values [13-14].

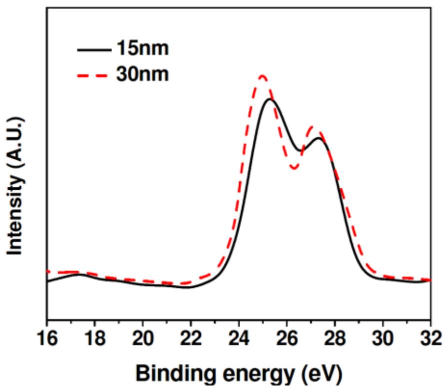

Fig.2. X-ray photoelectron spectra of TaN_x films at different thicknesses.

The SEM images of TaN_x films deposited with different thicknesses are shown in Fig 3. At lower thickness of 5nm the films exhibited patched type microstructure. As the films thickness increases very fine grains appeared and the patches were disappeared and there was no voids or cracks observed. On further increasing the films thickness to 30nm, the grains size increases without voids and cracks on the films surface. The films deposited at thickness of 15 and 30nm are exhibited dense structure. These type of densely packed microstructure films are most suitable for diffusion barrier applications.

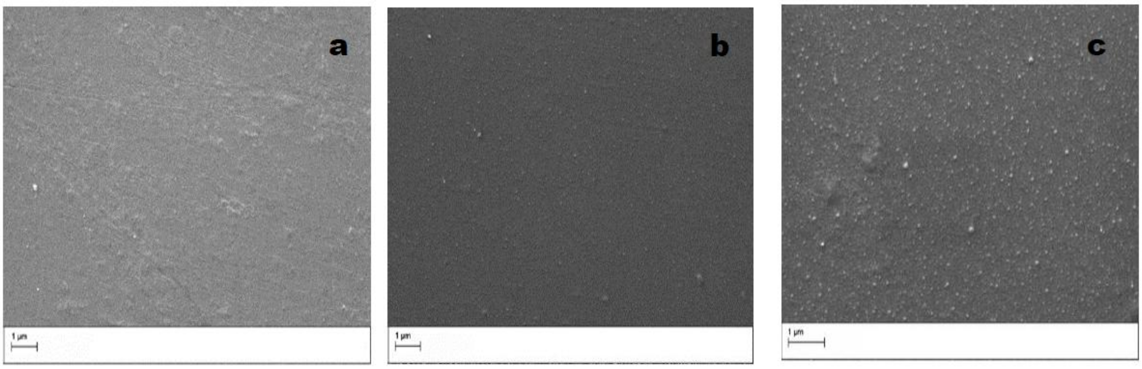

Fig.3. SEM images of ultrathin TaN_x films at different film thicknesses:(a) 5nm, (b) 15nm and (c) 30nm.

Fig.4. shows the two-dimensional AFM images of TaN_x films at different thicknesses. The films deposited at thickness of 5nm shows very fine grains with RMS surface roughness of 0.5nm. As increasing the films thickness grain size and the surface roughnesswas increased. The obtained RMS surface roughness of TaN_x films at 15 and 30nm are 0.7 and 1.3nm, respectively. This results suggest that the grain size becomes larger as the film gets thicker, and the roughness is associated with the grain size. Sun et al. [15] reported that the RMS roughness and grain size of dc magnetron sputtered ultrathin Al films increased gradually with increasing of films thickness. The increase of RMS roughness with films thickness mainly attributes to the increase of grain size.

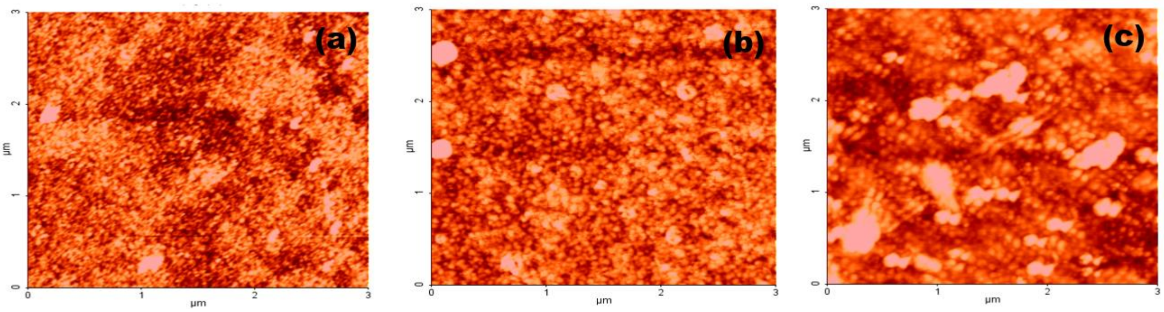

Fig.4. Two-dimensional AFM images of ultrathin TaN_x films at various film thicknesses: (a) 5nm, (b) 15nm and (c) 30nm.

The optical transmittance spectra of TaN_x films at different thicknesses were measured in the wavelength range of 300–1000nm and shown in Fig.5.The transmittance of bare glass was around 92% at wavelength of 550nm. The average transmittances of the films in the visible range increased from 88 to 91%with increases of film thickness from 5 to 15nm. Beyond this films thickness the transmittance decreased to 80%. The absorption edge was shifted towards lower wavelength side as increasing the films thickness. The variation of transmittance with films thickness was due to changes in microstructure and surface morphology of the films.

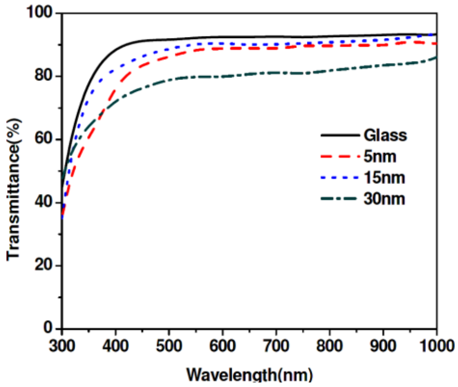

Fig. 5. Optical transmittance spectra of ultrathin TaN_x films at different thicknesses.

The optical band gap of the films wasstronglyinfluenced by the thickness and the band gap of the films was increased with increasing of the films thickness.The obtained band gap values are 2.62, 2.69, 2.84eV for the films thickness of 5,15 and 30nm, respectively. The obtained values are not near to the band gap values of Ta_2O_5 (Eg=4.5eV), TaO_2 (Eg=3.9-4.5eV), and Ta(NO) (Eg=4.3eV) [16-18]. This results indicate that the films deposited at different thicknesseswas not contained oxygen. The sheet resistance of the films was measured by using four-point probe technique and the as deposited films shows very high sheet resistanceregardless of films thickness.

IV. CONCLUSIONS

The effect of films thickness on the properties of ultrathin TaN_x films deposited on glass substrates by dc reactive magnetron sputtering were successfully investigated by XRD, XPS, SEM, AFM and UV-Vis-NIR spectrophotometer. X-ray diffraction results showed that the deposited films have amorphous structure. As the films thickness increases very fine grains appeared and the patches were disappeared and there was no voids or cracks observed. As increasing the films thickness grain size and the surface roughness was increased. The average transmittances of the films in the visible range increased from 88 to 91% with increases of films thickness from 5 to 15nm. The as deposited films shows very high sheet resistance regardless of films thickness.

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