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Fabrication and characterization of Al/Ta thin films as metal junctions for solar cell applications

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ABSTRACT

In the present work, the effect of deposition time (10 min, 20 min, and 30 min) on the structural, morphological, and electrical properties of Al/Ta thin films has been investigated. The XRD and microscopy results revealed that the thin films exhibit a bcc structure, with a strong (1 1 0) preferred orientation and followed a columnar growth with grain sizes lower than 100 nm. Thin film with 20-min deposition time exhibits less average roughness and better morphology than 10-min and 30-min. Further, the average resistance was smallest for thin films with 20-min of deposition time along with the optical reflectance between 50 and 85% in wavelength region of 400–1000 nm. The Al/Ta thin film can be employed as an excellent back-contact material for thinfilm solar cells due to its improved crystallinity, reflectance, and lower resistivity.

Introduction

Tantalum (Ta) is widely employed in the microelectronics industry owing to its outstanding corrosion resistance, ductility, high temperature stability, chemical inertness and favorable electrical characteristics [1–3] and Ta is most commonly found in the stable -Ta phase, which has a higher electrical conductivity and is less brittle than the metastable -Ta phase. Ta films exist in three phases: body centred cubic (α-Ta phase), tetragonal (β-Ta phase) and face centred cubic (FCC-Ta) face. The distinct Ta-phases generated are influenced by the deposition process and parameters, as well as layer thickness and substrate material [4–10]. It is well known that Ta-Al films exhibit excellent resistor stability [11,12] and Al-Ta alloy films have demonstrated excellent resistance to hillocks [13]. It has been reported that the DC magnetron sputtering produces a more uniform and stable coating devoid of dislocations and crystallographic defects in comparison to other types of magnetron sputtering [14].

We have investigated the influence of process parameters during the fabrication of DC magnetron sputtered Al/Ta thin films on the films structures, crystalline texture, and electrical properties using scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction spectroscopy (XRD), Energy dispersive X-ray (EDX) and four points probes (FPP). The structural and microscopy results show that the thin films exhibit a bcc structure, with a strong (1 1 0) preferred orientation and a columnar growth with grain sizes lower than 100 nm. The thin film with 20-min deposition time exhibits less average roughness and better morphology than 10-min and 30-min. The average film resistance (0.428 Ω/sq) was lowest for 20 min and exhibits good optical reflectance.

2. Methods and characterization

2.1. *Fabrication of film*

The substrates (glass) of size 1×1 cm^2 were ultrasonically cleaned with acetone and alcohol, then dried with nitrogen to remove surface contaminants before the deposition of thin films. The DC magnetron sputtering (Kur) was used to fabricate thin films on glass substrate under controlled growth conditions by adjusting deposition time (10, 20, and 30, minutes) [15]. Tantalum cylinder target (length of 20 cm and a radius of 3 cm; purity: 98%) was employed as a sputtering source. The vacuum pressure of the deposition chamber was ~10^{-6}torrs. The

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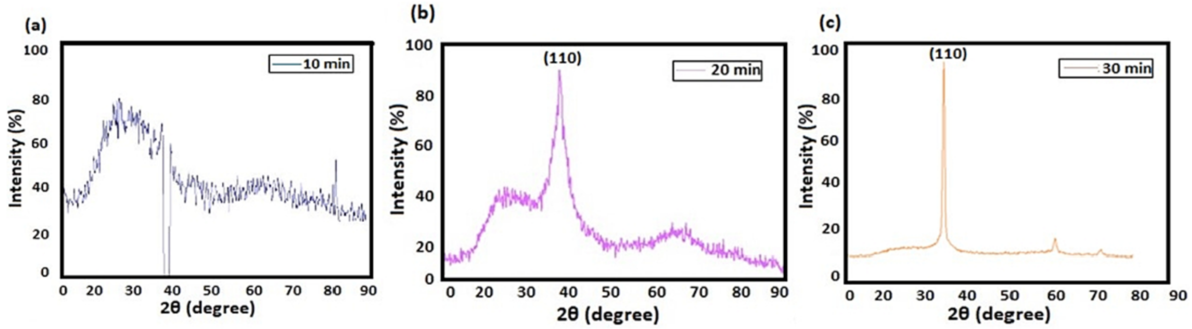

Fig. 1. XRD images of Al/Ta layer growth at different time interval of (a) 10 min, (b) 20 min, and (c) 30 min.

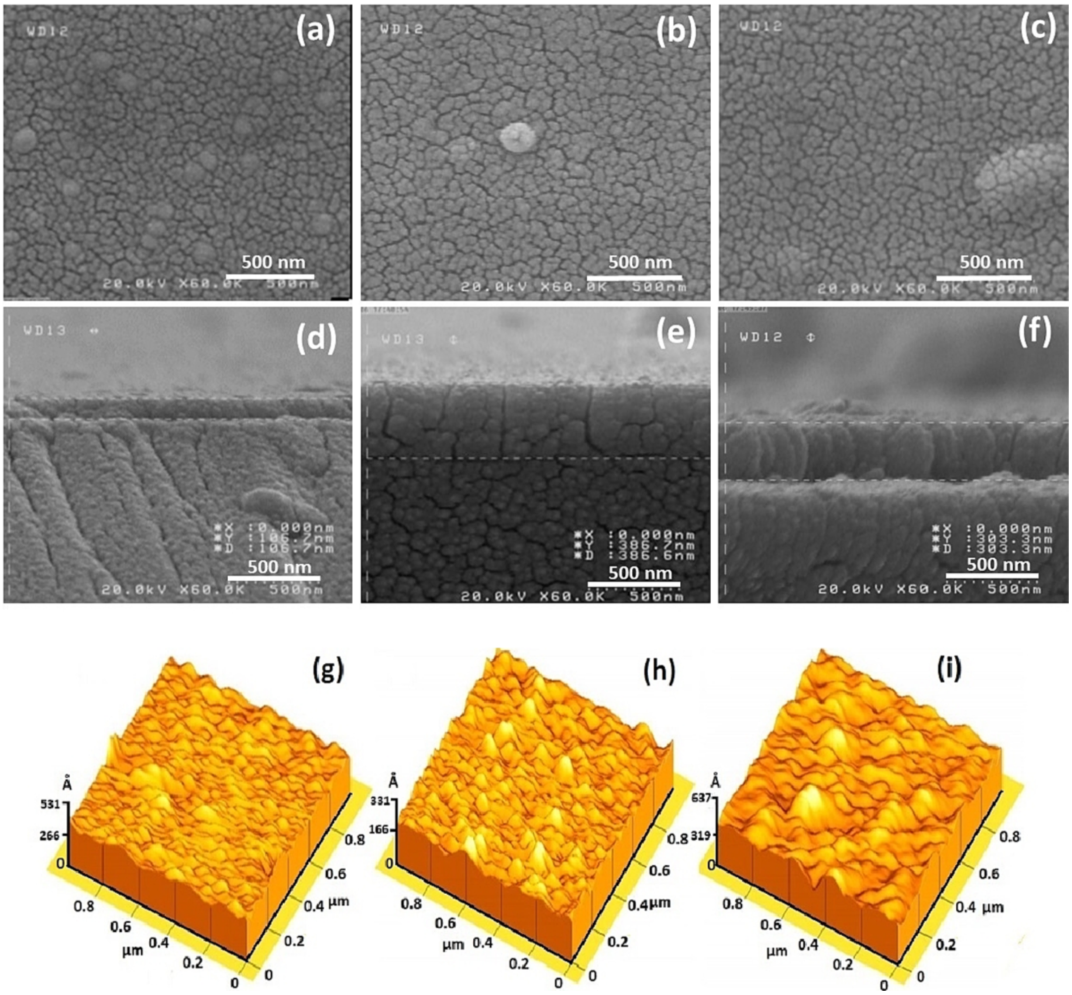

Fig. 2. SEM images of (a) 10 min (b) 20 min, and (c) 30 min deposition time along with the cross-sectional SEM images of (d) 10 min (e) 20 min, and (f) 20 min deposition time. AFM images of thin films fabricated at (g) 10 min, (h) 20 min, and (i) 30 min deposition time.

distance between target and substrate was set to 5 cm. With a flow rate of 80 sccm, argon gas with a purity of 99.99% was introduced. Cathode (target) was connected to a high-voltage power supply for ionizing argon gas and creation of plasma inside the chamber. DC power used for this experiment was set at 120 W. The ionized argon ions accelerated toward the cathode and sputter off the target material into the plasma. These sputtered target atoms impact energetically on the substrate (kept at room temperature) and gets deposited.

2.2. Characterization-

The thin films were investigated using a variety of characterization techniques, including XRD, FESEM, AFM, electrical analysis, and reflectance spectra. A scanning electron microscope (Hitachi S4160) was used to examine the morphology of the thin films. An XRD (STADI MP -Model) with Cu kα irradiation was used to investigate the structural properties of thin films. A dual-beam UV–vis spectrophotometer (Park scientific instruments atou probe cp and Cary 500 UV/VIS/NIR spectrophotometer) was used to measure reflectance in the 200–1000 nm spectral region. The electrical resistivities of all samples were evaluated

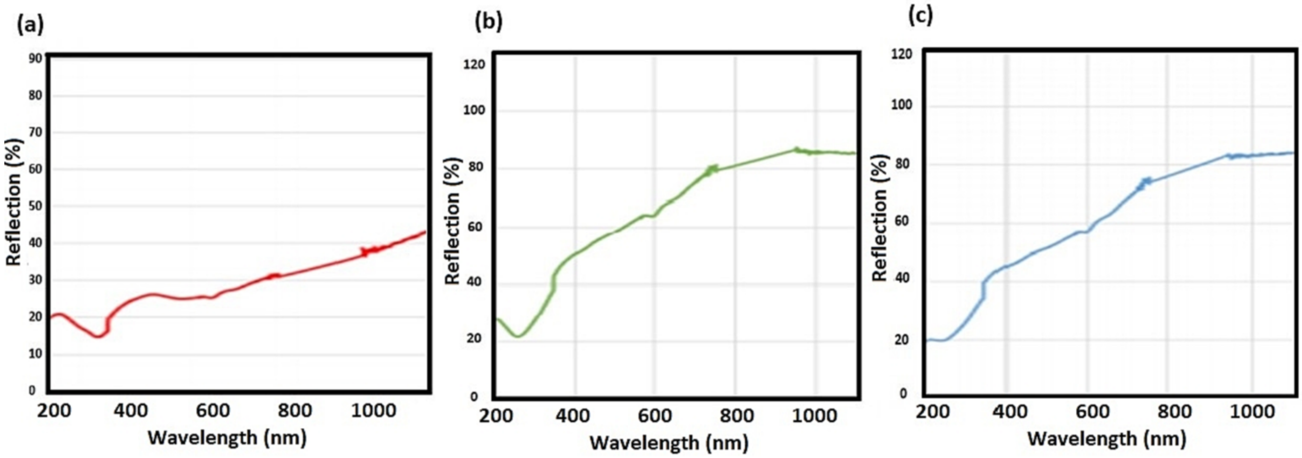

Fig. 3. Reflectance spectra of Al/Ta film with (a) 10 min, (b) 20 min, and (c) 30 min time of deposition.

using four-point probe (FPP) techniques (MELLER). The roughness of the thin films was determined using AFM (Park scientific instruments atou probe cp).

3. Results and discussion-

a) Structural studies

The XRD profile of as-deposited Ta/Al thin films at three deposition time 10, 20, and 30 min in the scanning range of 2θ from 20-90^0 is shown in Fig. 1[11]. The diffractrogram for Ta/Al thin film at 10 min deposition time represent their amorphous growth as there is no Al peak (~38°) present in XRD data, Fig. 1 (a). With increase in deposition time to 20 min, a small reflection peak at 37.9° appeared, which represent nanocrystalline formation with an amorphous background. Some other peaks are also appearing at 20 min deposition time represent orthorhombic structure as shown in Fig. 1(b). But At 30 min deposition time Ta/Al thin film shows a weak diffraction peak at ~ 69° and ~ 81°, Fig. 1 (c), suggesting that the films are cubic polycrystalline.

The crystal size was calculated from the Scherer equation [16]. For 10, 20, and 30 min of deposition, observed FWHM is 0.6298, 0.6298, and 0.6691, respectively, with peak position 38.47°, 38.92°, and 38.67°, respectively. The calculated crystallite size comes out to be 13.36 nm, 13.34 nm and 12.56 nm for 10-, 20-, and 30-minutes deposition time, respectively.

b) Surface morphology

SEM micrographs display the microstructure of Al/Ta thin films fabricated at deposition time of 10, 20, and 30 min, as shown in Fig. 2 (a)-(f). It can be observed from Fig. 2(a), and (d) that for 10 min only initial germination and islands are formed with small thickness of 100 nm. With increase in the deposition time to 20 min, a uniform layer formation can be observed with average thickness of 400 nm, Fig. 2 (b), and (e). Further on increasing deposition time to 30 min, leads to decrease in the film thickness to 300 nm, Fig. 2 (f). This can be attributed to splitting of few layers of the deposited film with impact of target ions for increased deposition time. This may be due to the self-limiting growth of thin film governed by a smaller number of available reaction sites on the substates, where the target ions no longer get deposited.

The AFM measurements for 10 min deposition time, shows a rms roughness of 26.2 Å, Fig. 2 (g). In case of 20 min, the rms roughness size decreased to 19.5 Å, Fig. 2 (h) suggesting a smooth film formation. The decrease in roughness is due to grain growth mechanism and agglomeration of smaller grains and surface reactions. With further increase in the deposition time to 30 min, the rms roughness increased to 44.4 Å, Fig. 2 (i), which is in agreement with SEM results.

EDX spectroscopy revealed the elemental stoichiometry of a 20-minute deposition film where Al (11.32%) and Ta (70.30%) are present with just trace amounts of carbon (8.85%) and oxygen (4.08%). The percentage of reflection was observed between 35 and 40%, 50–85%, and 45–82% for 10 min, 20 min, and 30 min of deposition time for wavelength region 400–1000 nm, Fig. 3 (a)-(c). Since a high reflection in a metal contact of a solar cell is required, so the thin films with in 20-minutes and 30 min of deposition time can be used.

In the case of 10 min of deposition time, the measured electrical resistance was high (2.74 Ω/sq), which is due to lack nonuniformity of the thin films. For 20 min, the electrical resistivity was measured to 0.428 Ω/sq, which shows a considerable decrease in resistance due to uniformity of Al/Ta film. For 30 min deposition, the resistance was measured to 0.487 Ω/sq. This small increase in resistance (by 0.6 Ω/sq) can be attributed to the non-uniformity and high roughness of the film. Thus, we conclude that the sample with 20 min of deposition is a better choice because of its less electrical resistance.

4. Conclusion

In this paper, growth and physical characteristics of Al/Ta thin films deposited by DC magnetron sputtering as a function of deposition time (10 min, 20 min, and 30 min) have been studied. The XRD analysis reveals that the grown thin films for 10 min of deposition time were devoid of Al content. In case of 20 and 30 min of deposition time, a bcc structure, with a strong (1 1 0) preferred orientation with crystal size of 13 nm was observed. The SEM analysis revealed that thin film with 20 min of deposition time has the best uniform morphology with average thickness of 400 nm among two other deposition time of 10 and 30 min, further supported by AFM analysis. The electrical resistance was found to be least (0.428 Ω/sq) for the 20-minute. Further, the thin film with 20-minute deposition show good optical reflectance (50–85%) in the wavelength region from 400 to 1000 nm. Thus, the Al/Ta thin films with 20-minute deposition duration can be offered as a suitable candidate for back contact in solar cell applications.

CRediT authorship contribution statement

Kamil Monga: Data curation, Formal analysis. **Larak Labbafi:** Conceptualization, Data curation, Formal analysis. **Harshita Trivedi:** Investigation, Methodology, Writing – review & editing. **Zohreh Ghorannevis:** Project administration, Supervision, Resources. **Avanish Singh Parmar:** Conceptualization, Supervision, Writing – original draft. **Shilpi Chaudhary:** Writing – original draft, Resources, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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