

TOWARDS THE FABRICATION OF FLEXIBLE THIN FILM CdTe SOLAR CELLS: THE SIGNIFICANCE OF SUBSTRATE SURFACES

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ABSTRACT

Thin film CdTe solar cells have been recognized as reliable alternative for the manufacture of cheap photovoltaic solar cells of the future, due to its excellent absorber characteristics and simple, low-cost manufacturability. However, for the attainment of higher cell performances, additional studies are needed to increase cell efficiency through further development of better quality films and new fabrication processes. In the *substrate-structured* CdTe thin film solar cells, the CdTe absorber layer is deposited directly onto the substrate or through a back contact layer. But the quality of deposited film is believed to depend on the type and smoothness of the substrate. In this work CdTe was deposited on different substrates by RF sputtering and the effects on the deposited films were studied in terms of their structural and morphological forms. The substrates used were: pure molybdenum sheets (Mo), molybdenum-sputtered on molybdenum (Mo/Mo), molybdenum-sputtered polyimide (PI/Mo) and molybdenum-sputtered glass (glass/Mo). The characterization tools used included XRD, SEM and AFM. The results showed that all surfaces produced uniform, compact and pinhole-free films; however, those on smoother surfaces produced larger as-deposited grain sizes of up to 1.7 μ m as against 1.3 for rougher surfaces. Non-uniformities such as overgrowth and voids were observed, but only films on PI showed evidence of cracking and peel-offs.

Keywords: CdTe, substrate, molybdenum, polyimide, thin film, surface roughness.

INTRODUCTION

The development of low cost photovoltaic solar cells has found thin film technology as an appropriate and suitable vehicle for the global transfer from fossil-based energy sources to an affordable and environmental friendly photovoltaic (PV) renewable energy sources. Thin film solar cells have the advantages of simpler, cheaper and faster deposition processes and equipment, compared to traditional crystal silicon based solar cell technology. Amongst the thin film solar cells CdTe and CIGS types have shown attractive features with CdTe having the largest PV industrial production by first Solar which produced 12.1 GW of module with an efficiency of 22.6% which is expected to rise by 2 GW by 2026 (First Solar, 2024, Scarpulla et al. 2023). Nevertheless, for such cells to compete favorably with conventional fossil sources there is strong need to reduce production cost and increase cell efficiency. One of the ways of achieving these is through improving the quality of films deposited during cell fabrication. An important step in this direction is in understanding the effects of various substrates on the quality of deposited films. Although it is believed that smoother surfaces produce better quality deposited films than rough surfaces, but this has not been fully investigated. In conventional superstrate-structured CdTe solar cells, films are deposited on

glass, having smooth and flat surfaces. However for substrate structure, such as in flexible solar cells, such advantage is not readily at hand because the CdTe is deposited directly, or through a back contact layer, onto polymer or metallic sheets with rougher surfaces. In addition, during the back contact fabrication, different materials and deposition strategies are applied, in order to obtain good Ohmic contact. These may lead to unwanted effects due to surface variation. Thus special considerations need be taken to overcome this issue. For CdTe based flexible thin film solar cells, molybdenum has been identified as the most suitable material for the substrate structure. Among the reasons for its choice include its readily availability in high purity form as well as its excellent matching of coefficient of thermal expansion (CTE) to that of CdTe (Singh et al. 1999), which (Hodges 1999) showed, determines the flaking, delamination and adhesion of films in flexible substrates. A smooth substrate is considered necessary for several reasons (Drayton et al. 2005), among which are: 1. Rough surfaces, with their spikes and cavities may lead to non-uniformities in deposited films as well as pin holes and consequently shunts between the front and back contacts. 2. Surface roughness strongly influences the properties of subsequent layers such as growth and crystal orientation. 3. The deposition of buffer layers such as back surface field (BSF) may be easier and more successful on smoother surfaces. Hodges (2009) showed that the growth of CdTe morphology strongly depends on the type of substrate smoothness, while (Batchelor et al. 2009) and (Wuerz et al. 2011), each showed that solar cell performance indices (J_{sc} , Voc, FF and η) all improve with smoother substrates.

In this work, we investigated the significance and effects of different surface conditions on the film quality and possible effects on the performance of CdTe solar cells. A new approach proposed here was to sputter Molybdenum on Molybdenum sheets in order to smoothen out the possible rough surface. Sheets of Molybdenum (Mo), polyimide (PI) and sodalime glass (GI) have been used as substrates, by sputtering a thin layer of Mo each, as a back contacting layer as well as to modulate the surfaces of these substrates. The resultant films of CdTe were also deposited by RF sputtering and then characterized in order to study their structural, morphological, grain sizes and roughness as well as their possible impact on deposited film.

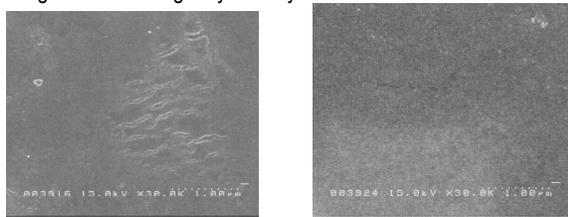
MATERIALS AND METHODS

Thin sheets of Mo, PI and soda lime glass were cleaned in ultrasonic bath using the 3-stage acetone-ethanol-DI water for 5 minutes each, followed by drying using nitrogen gas. Next, Mo target of 99.95% purity was sputtered onto these substrates to a thickness of about 400-500nm. The sputtering chamber was evacuated to a base pressure of 1.7×10^{-4} Torr while the sputtering conditions were: RF power of 100W, substrate temperature of

200°C, and argon pressure of 1.2 mTorr. Then another cleaned Mo sheet was added to these and CdTe films were also deposited by sputtering. Using XRD, SEM and AFM the films were characterized and their possible effects on solar cell fabrication investigated.

RESULTS AND DISCUSSION

From the SEM, presented in Fig. 1 (a) and (b), we compare the surfaces of the Mo sheet and Mo sputtered-Mo (Mo/Mo), under same magnification. It is readily observed that while the Mo sheet has rough surface with obvious 'craters' and 'bumps'. However, when Mo was sputtered these were covered up and smoothed out. From the XRD signatures of the two surfaces presented in Fig. 2, the molybdenum in each case appears to form in 2 phases; while for Mo the peaks appear at 57.94° and 73.08°, for Mo/Mo they are at 58.52° and 73.58° respectively. These have been identified as the (200) and (211) orientations respectively (Roosz, 2010). These images show the high crystallinity of the films.



(a) Mo sheet (b) Mo sputtered on Mo (Mo/Mo)
Figure 1. SEM images of different molybdenum surfaces

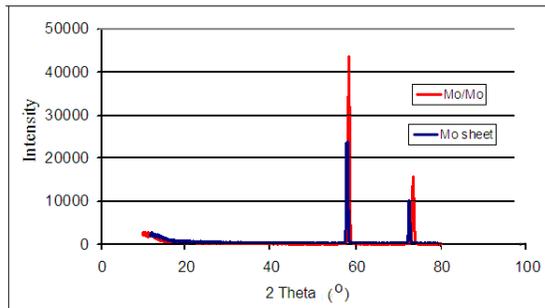
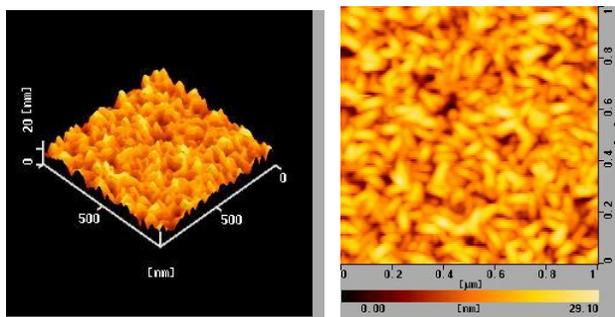


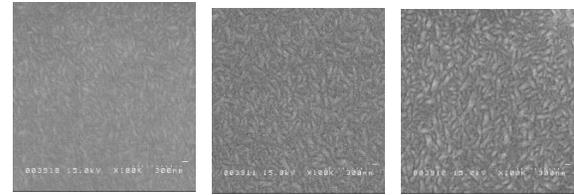
Figure 2. XRD of molybdenum sheet and sputtered molybdenum



(a) Glass/Mo surface in 2-D (b) After corrections
Figure 4. AFM images of Surfaces

On the other hand, voids and cracks have been observed in the PI/Mo/CdTe films. These cracks are common problems of CdTe films deposited on flexible substrates, most especially polymer materials, due to their brittleness at elevated conditions such as temperature, plasma bombardments and pressure. Special care

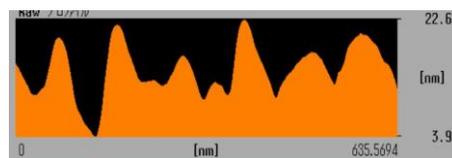
For comparison, the SEM of Mo films on all the 3 surfaces (Mo, glass and PI) are presented in Fig. 3, at higher magnification of 100k. It is readily observed that while all the deposited films were smooth, compact and uniform, these film qualities follow the order of the surfaces' smoothness. Thus, glass, with the smoothest surface, gives the best films while Mo has roughest surface. The AFM images of Glass/Mo of Fig. 4 further proves the good morphology of this film. The roughness index was found to be in the range 3.20-3.22nm with RMS values of 4.00-4.03nm.



(a) Mo/Mo (b) PI/Mo (c) Glass/Mo
Figure 3. Sputtered Mo on different substrate surfaces

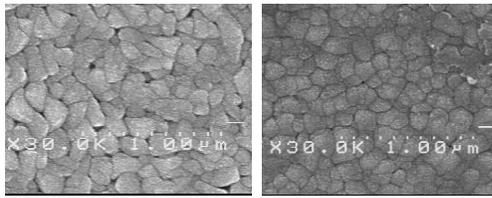
Next, the SEM close up of the CdTe films on both PI/Mo and Mo sheets as presented in Fig. 5 show the fairly large grains of the as-deposited films. Both films have compact, large grains and uniform distribution, with no signs of pinholes. The average grains size of the as-deposited films on PI of 1.5 is slightly higher than that on Mo with 1.3 μm. This may be attributed to the smoother surface of the PI substrate. Large grain size CdTe films are important in the fabrication of high efficiency solar cells by reducing carrier recombination, thereby improving cell efficiency (Ohring, 1992).

Some interesting abnormalities in film growth were observed as captured by the CdTe SEM in Fig. 6. The *cornflower* and other overgrowths were observed, in the Mo/CdTe and PI/Mo/CdTe films (a) and (b). They were as result of new nucleating points on the film, arising due to variations in the deposition conditions such as temperature and plasma properties [11]. Moreover, Nucleation and growth stages are dependent upon various deposition conditions, such as growth temperature, growth rate, and substrate chemistry (Wasa, 2004).

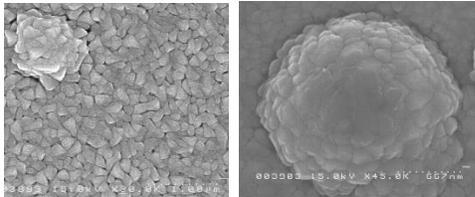


(c) Roughness of Glass/Mo

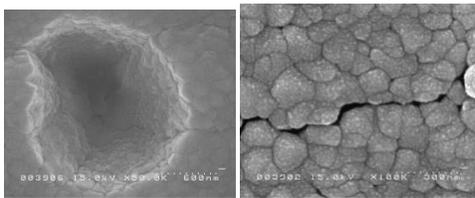
need be given during deposition and handling of these samples.



(a) Mo/CdTe/CdS (b) PI/Mo/CdTe/CdS
Figure 5. SEM of CdTe/CdS on flexible substrates



(a) Cornflower (b) Overgrowth



(c) Void (d) Cracks

Figure 6. Non-uniformities in growth

Conclusion

The influence of substrate on the quality of subsequent layers deposited in substrate structure of CdTe thin films has been investigated and their possible effects on solar cells discussed. By using 4 different materials of varying surfaces, the structural and morphological forms of the deposited CdTe films showed that compact, uniform and pinhole-free films are obtainable. However, it was observed that smoother surfaces produce slightly larger grain sizes compared to rougher surfaces. Thus, it was shown here that by sputtering molybdenum on molybdenum sheets, the rough surface was smoothed out, leading to better film quality. Meanwhile, films on polyimide showed deposition non uniformities such as overgrowth, voids and severe cracks and peel-offs, while films on molybdenum exhibited cornflower overgrowth. These later film behaviours could have negative effect on the performance of thin film solar cells, as they create discontinuities, voids and centres of recombination. Thus, substrate surface plays significant role in substrate structure CdTe solar cells. Further studies on the effects of these on the actual performance indices of the cells are being carried out.

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