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Effect of a TiN alkali diffusion barrier layer on the physical properties of Mo back electrodes for CIGS solar cell applications

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ABSTRACT

$Cu(In,Ga)Se_2$ thin-film solar cells have attracted strong interest in the photovoltaic community due to their high efficiency and demonstrated industrial relevance. As the most commonly used back electrode for CIGS solar cells, molybdenum (Mo) is typically deposited on soda-lime glass substrates by magnetron sputtering. During the high-temperature CIGS absorber formation process step, alkali (Na) atoms diffuse from the soda-lime glass substrate into the CIGS absorber via the Mo contact, a process that is known to improve the cell efficiency. However, Na diffusion from soda-lime glass sheets is an uncontrolled process, which adds to batch-to-batch variations due to fluctuations in the glass quality and process parameters such as the CIGS formation temperature. Hence, a diffusion barrier layer between the glass substrate and the Mo back electrode is required to prevent this uncontrolled impurity diffusion. In this study, a TiN diffusion barrier layer is deposited by reactive magnetron sputtering of a metallic Ti target, using various N_2 flow conditions. It is observed that the adhesion, microstructure, and morphology of the Mo films get significantly improved by the introduction of a TiN barrier layer, which in turn leads to better cell efficiencies. Hence, the TiN/Mo bilayer design developed in this work seems to be a good choice for enhancing the efficiency of CIGS solar cells.

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1. Introduction

Copper indium gallium di-selenide [$Cu(InGa)Se_2$ (CIGS)] and related chalcopyrite compound solar cells have attracted strong interest in photovoltaic (PV) research and applications due to their high efficiencies. Recently, there have been large efficiency improvements for CIGS solar cells prepared both on flexible polymer and rigid glass substrates. Using a flexible polymer substrate EMPA in Switzerland reported 20.4% cell efficiency, while on rigid glass substrates ZSW in German reported 22.6% efficiency, which exceeds that of the market dominating multicrystalline silicon solar cells [1–3]. This substantial progress in CIGS solar cell efficiency has been attributed to a new alkali element doping procedure, i.e. the alkali post-deposition treatment (PDT) of the absorber layer. Although there still lacks clear evidence to exactly explain the role and chemical environment of alkali doping, the CIGS devices were proven to benefit from the optimized alkali element doping in several ways: decreased resistivity of the p-type CIGS layer, increased fill factor (*FF*) and open-circuit voltage (V_{oc}), and reduced recombination losses at the surfaces of the CIGS absorber [1,4–8]. However, the amount of alkali dopants should be kept below 0.1 at. % in the CIGS absorber [9–11]. An excessive amount of alkali dopants was reported to have negative impacts on the efficiency and the long-term stability of CIGS solar cells, and can even cause potential induced degradation (PID) of the cells [12–15].

Several strategies have been proposed to incorporate alkali atoms into CIGS absorbers. Each method has its own merits and demerits. The most widely used utilizes an internal sodium source - the soda-lime glass (SLG) substrate - for sodium diffusion through the molybdenum (Mo) back contact, which is the most economical and simplest method. However, it is difficult to accurately control the sodium content in the SLG substrates. The sodium content in SLG varies from batch to batch, and even shows a non-uniform distribution across the width of each substrate [16]. In addition, the sodium diffusion into the CIGS absorber depends on the microstructure of the Mo layer deposited onto the glass substrate. In contrast, incorporation from an external source, like deposition of an alkali-containing layer and alkali PDT, is a more controllable technique for alkali doping. However, when the substrate contains

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alkali elements or harmful impurities, a diffusion barrier layer between the substrate and the Mo rear contact is needed for precise control of alkali doping of CIGS absorber layers [17–19].

The barrier layer materials used so far include metals (Cr, Ta), oxides, nitrides and oxynitrides [17,18,20–26]. Among these, a TiN thin film deposited by reactive magnetron sputtering is one of the most promising diffusion barrier layers for PV applications [17,27,28]. However, the properties of TiN films depend strongly on the deposition conditions, which can significantly affect the microstructure and also the crystallographic orientation of TiN films. The microstructure evolution of the TiN can be depicted in term of structure zone model (SZM) [24,29]. For diffusion barrier layer applications, a TiN film with V-shaped columnar structure is considered as the best choice [29]. In order to grow V-shaped TiN films, the deposition condition should be optimized.

In this work, TiN thin films are deposited by reactive direct current (DC) magnetron sputtering, as a barrier layer between the SLG substrates and the Mo thin films. The effects of the N_2 gas flow on the microstructure of the TiN thin films are investigated. The microstructure and surface morphologies of the Mo back contact with TiN barrier layer are studied with respect to fabricating advanced back contacts for CIGS solar cells. Furthermore, we demonstrate that the newly developed TiN barrier layer can also serve as an adhesion improvement layer.

2. Experiments

2.1. Sample preparation

TiN thin films were deposited onto A3 size (40 cm × 30 cm) SLG substrates by reactive DC magnetron sputtering (Line540 system from FHR Anlagenbau GmbH, Germany) using a planar metallic titanium target (purity 99.99%, size 540 mm × 90 mm) in an Ar-N_2 environment. The working gas flow (Ar, purity 99.999%) was kept constant at 120 sccm and the reactive gas flow (N_2, purity 99.999%) varied from 0 to 8 sccm, while the chamber pressure was kept approximately constant at 3.0×10^{-3} mbar. Two sets of TiN films with different thicknesses of 90 and 210 nm were deposited for different characterization purposes. Mo films were deposited onto the 210 nm thick TiN films using a metallic planar Mo target (purity 99.99%, size 540 mm × 90 mm). During deposition, both the power applied to the target and the chamber pressure were kept constant at 2 kW and 1.5×10^{-3} mbar, respectively. All sample depositions were conducted at room temperature without any substrate heating. The deposition was carried out in dynamic mode (i.e., multiple pass deposition). During deposition, the SLG substrate was vertically attached (i.e., portrait format) onto a moving carrier and allowed to oscillate in front of the cathodes at a constant speed of 10 mm/s for 3, 7 and 18 times, respectively, which resulted in 90 and 210 nm thick TiN layers and 900 nm thick Mo films. The deposition conditions of these films are summarized in Table 1. The Mo films with a TiN barrier layer and standard bilayer Mo rear contacts [30,31] were utilized to prepare CIGS solar cells. Multilayer CuGa(75:25 wt%)/In/CuGa/In stack design was used to prepare the Cu-In-Ga precursor. The selenization of the precursor was performed in nitrogen atmosphere at ambient pressure using an inline rapid thermal processing (RTP) furnace supplied by the Smit Thermal Solutions, Netherlands. The heater temperatures of the RTP were 580 °C and the duration of the high temperature process was about 12 min. Thermally evaporated (420 °C) Se vapour was used as the Se source to form CIGS absorber layer. There are many advantages in using elemental Se vapour other than toxic H_2Se as Se source such low cost, easy-handling and less absorber process time. Highly resistive intrinsic ZnO films and conductive aluminium-doped ZnO (AZO) films were deposited by RF and DC magnetron sputtering, respectively, acting as the window layer and front electrode. Finally, Ag/Al finger contacts were deposited by DC magnetron sputtering to reduce resistive losses.

2.2. Sample characterization

Several characterization methods were used to analyze the TiN and Mo films. The film properties such as density (ρ), thickness (d) and surface roughness (σ) values were derived from X-ray reflectivity (XRR) measurements performed at the X-ray demonstration and development (XDD) beam line at the Singapore Synchrotron Light Source (SSLS) [33]. The experimental XRR curves are theoretically simulated with the LEPTOS software to derive the film properties [34]. The four-point probe method in the van der Pauw configuration was used to measure the sheet resistance of the samples. The thickness of the TiN and TiN/Mo films deposited on glass substrates were measured by a stylus profiler. Grazing angle X-ray diffraction (GXRD) measurements were conducted to understand the crystal structures of the 210 nm thick TiN films and TiN (210 nm)/Mo (900 nm) stacked films. The grain size (D) along the preferred orientation of the deposited films was estimated via the Scherrer equation:

$$\textit{Grain size}\ (D) = \frac{0.9\lambda}{\beta\cos\theta} \quad (1)$$

where λ, β and θ are the wavelength of the X-ray (Cu $K\alpha_1$), the full width at half maximum (FWHM) and the Bragg diffraction angle, respectively. The surface morphologies of the 210 nm thick TiN and TiN (210 nm)/Mo (900 nm) films were measured by atomic force microscopy (AFM; Veeco, NanoScope D3100) and scanning electron microscopy (SEM; Carl Zeiss, Auriga-39-35). The performance of the CIGS solar cells prepared on this modified Glass/TiN/Mo back electrode was measured under standard one-sun illumination conditions using a LED-based solar simulator (Sinus 220, Wavelabs, Germany).

3. Results and discussion

3.1. Optimization of TiN barrier layer

3.1.1. Hysteresis loop

It is well documented that, during reactive magnetron sputtering processes, the target materials react with the reactive gas not only on the surface of the substrate (thereby forming a compound coating film) but also all over the target and the chamber walls [35]. A hysteresis loop occurs due to the formation of reactive products

Table 1
Deposition conditions of TiN and Mo films by magnetron sputtering.

Samples	Thickness (nm)	Power (kW)	Power density (W/cm^2)	Ar (sccm)	N_2 (sccm)	Pressure (mbar)	Substrate temperature (°C)
TiN	90	2	4.36	120	0, 2, 3.5, 6, 8	3×10^{-3}	25
TiN	210	2	4.36	120	3.5, 6, 8	3×10^{-3}	25
Mo	900	2	4.36	80	0	1.5×10^{-3}	25

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