

Above 14% efficiency earth-abundant selenium solar cells by introducing gold nanoparticles and Titanium sub-layer

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ABSTRACT

In this paper, a new Selenium (Se) solar cell design based on inserting dissimilar ultrathin metallic layers (MLs), (Au and Ti), is proposed. Analytical models of the proposed design are developed, where the analytical results are in agreement with the experimental data. In addition, the role of the introduced ultrathin MLs in enhancing the light-scattering in the Se solar cell structure is also demonstrated. Moreover, the impact of the Mg mole fraction of the ZnMgO buffer layer on the device performance is investigated. It is revealed that the proposed structure give rise to optical micro-cavity effects which leads to improve the absorbance and reduce the reflection. Genetic Algorithm (GA) technique is used to boost up the solar cell efficiency by selecting both the appropriate position of the ultrathin MLs and the suitable Mg mole fraction of the ZnMgO layer. It is concluded that the optimized design with Ti MLs pinpoint a new path toward achieving superior power efficiency of 13.2%, where improved I_{sc} of 21 mA/cm² and enhanced V_{oc} of 1 V are recorded. Moreover, the impact of the metallic nanoparticles (MNPs) introduced in the ZnMgO buffer layer on the device performance is also investigated, where an improved power efficiency value of 14.7% is recorded. This makes the optimized designs potential alternative top cells for developing high-efficiency tandem photovoltaic devices at a reasonable cost.

1. Introduction

Recently, photovoltaic energy has emerged as a compelling solution to meet the world's increasing requirements of clean and sustainable energy [1,2]. As a matter of fact, concerns about the elaboration cost of the photovoltaic cells, as well as their conversion efficiency, have limited the deployment of these energy resources [3–5]. In the 1980's, researchers have demonstrated the ability of the Se-based solar cell for providing a power efficiency of 5.0% [6,7]. However, this value remains far from the theoretical limit of the Se-based solar cell efficiency which is considered about 24% [6–9]. This is mainly due to various issues associated with the recombination and optical losses. Moreover, the enormous progress of the silicon microelectronic industry has motivated the researchers to focus on developing Si-based solar cell, which has led to achieve an excellent efficiency value of 26.6% [9]. In this context, achieving further improvement regarding the Si-based solar cells is extremely challenging since we are oncoming to their practical limits. This has led to explore alternative solar cell designs that might offer the potential to exceed the Shockley-Queisser limit. Tandem solar cell consisting of different materials with optimized energy band-gap can pinpoint a new path toward avoiding the problems of single

junction based-solar cells [10–14]. However, till now tandem technology has been restricted to low-efficiency hydrogenated Si (*a*-Si:H) and expensive III-V alloys solar cells. In this perspective, achieving high cost/efficiency ratio inevitably involves the exploration of alternative earth-abundant materials with good absorption characteristics. Accordingly, the major problem that prevents achieving high-performance multi-junction photovoltaic devices resides on the lack of an effective high band-gap top cell [13–15]. Over the last few years, attempts have experienced so far to address these issues by inserting several top cells based on perovskite, *a*-Si:H and even organic materials [16–18]. Potentially, perovskite material with high and suitable band-gap value of 1.6eV seems suitable for improving the tandem solar cell efficiency. However, stability and degradation related ageing effects associated with the perovskite compound are considered as the most pronounced challenges for its eventual use as a top cell in multi-junction technology. Thus, a fully transition to more stable and low-cost materials remains of great importance, which can open up a new way toward achieving high-performance photovoltaic cells. Selenium material with an appropriate band-gap of 1.95eV can be a promising alternative as an absorber region of the top cell. Despite these advantages, Se-based solar cells are unable to exceed 5% of efficiency. Recently, intensive efforts

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have been conducted to improve the world's oldest photovoltaic cell based on *Se* material through proposing a new redesigned architecture based on *ZnMgO/Se/MoO₃/Al* structure that can offer 6.5% of power efficiency [19]. Although this achievement, further improvements are in fact required in order to develop high-efficiency tandem solar cells. The deep knowledge of the interface properties and the main reasons behind the solar cell degradation is an important issue to identify the appropriate materials combination that allows enhancing the *Se*-based solar cell performance. To the best of our knowledge, no design approaches based on introducing intermediate ultrathin *MLs* (*Au* and *Ti*) and device global optimization were reported to reach promising effectiveness for boosting up the efficiency of the *Se*-based solar cell. For this purpose, we propose in this paper a new approach based on introducing ultrathin *MLs* within the *Se* absorber layer in order to enhance the solar cell light-scattering behavior. A comprehensive analytical model of the *Se* solar cell power efficiency is developed, where a good agreement with the experimental results is achieved. The effect of the inserted *MLs* on the photocurrent is analyzed. The impact of the *Mg* mole fraction on the solar cell performance is also investigated. Moreover, a new hybrid approach based on the analytical modeling of the proposed *Se*-based solar cell with ultrathin *MLs* and *GA*-based meta-heuristic computation is proposed. The merit of this approach is to properly engineer the absorber layer in order to generate optical confinement regions to achieve an improved absorption and avoid antireflection effects. In addition, the effect of gold *MNPs* introduced in the *ZnMgO* buffer layer on the *Se*-based solar cell performance is also investigated. The proposed structure offers the opportunity for improving the *Se* solar cell efficiency, which makes it a potential alternative top cell for providing high-performance tandem photovoltaic devices.

2. Modeling of the *Se*-based solar cell with ultrathin *MLs*

Basically, the key idea behind inserting ultrathin *MLs* inside the *Se* absorber region is to modulate the absorption behavior of the investigated *Se*-based solar cell and achieve encouraging power efficiency values. In this framework, the investigated design is considered with *ZnMgO/Se/Metal/MoO₃/Al* structure in which different ultrathin *MLs* such as *Au* and *Ti* are incorporated in our investigation. Fig. 1 shows the schematic of the proposed *Se*-based solar cell, where the *MLs* are introduced in the *Se* absorber region. This would be beneficial for reducing the optical losses through generating the resonant optical micro-cavity effect. The analyzed *Se*-based solar cell design is suggested with

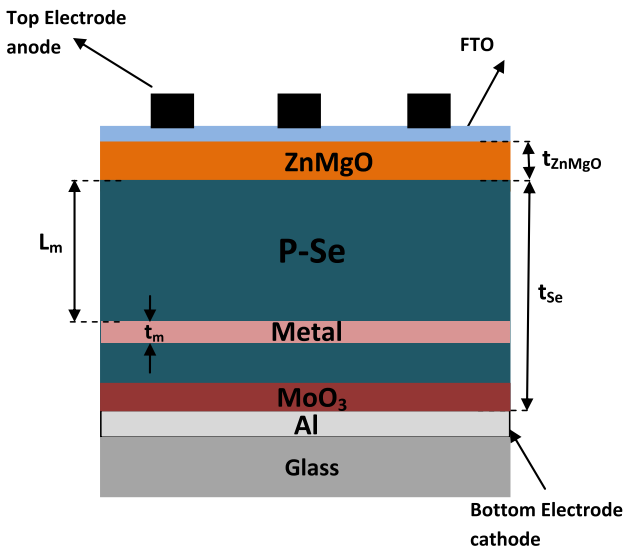


Fig. 1. Cross-sectional view of the proposed *Se*-based solar cell with intermediate ultrathin *MLs*.

P–N heterojunction ultrathin structure, where the *n-ZnMgO* layer behaves like a buffer region, while the absorber *P*-type region is suggested with *Se/MLs/Se* structure. On the other hand, a thin *MoO₃* layer is introduced at the bottom of the cell in order to reduce the recombination losses at the back contact. Moreover, the *Mg* mole fraction plays an important role in determining the quality of the *Se/ZnMgO* interface as well as the separation mechanism of the photo-generated carrier.

As it is illustrated in Fig. 1, the parameter t_{Se} denotes the thickness of the *Se* absorber layer, t_{ZnMgO} represents the *ZnMgO* buffer layer thickness, t_m and L_m are respectively, the thickness and position of the inserted *MLs* with respect to *Se/ZnMgO* interface.

In order to model the *Se*-based solar cell, we need to develop the analytical current-voltage formulation of the proposed *ZnMgO/Se/Metal/MoO₃/Al* structure by incorporating the effect of the inserted ultrathin *MLs*. In this context, the well known current-voltage expression of the conventional solar cell under illumination is exploited [20].

$$I(V) = I_{ph} - I_s \left[e^{\frac{V - IR_s}{nV_{th}}} - 1 \right] - \frac{V - IR_s}{R_{sh}} \quad (1)$$

where, q denotes the electron charge, V_{th} is the thermal voltage, R_{sh} and R_s are respectively, the shunt and series resistances, I_s represents the saturation current, I_{ph} is the photocurrent and n refers to the ideality factor.

The first step toward extracting the current-voltage characteristic of the investigated *Se*-based solar cell designs is to estimate the photocurrent delivered by the adopted *ZnMgO/Se/Metal/MoO₃/Al* structures with and without ultrathin *MLs* under illumination. To do so, we should accurately calculate both absorbance and reflectance optical parameters for the investigated designs. In this framework, the *ATLAS-2D* device simulator with *2-D LUMINOUS* module is used for the discretization of Maxwell's equations by means of the *FDTD* method. This device simulator is regarded as a powerful tool for modeling the solar cell optical behavior [21].

The modeling procedure and the computation methodology used to calculate the optical parameters associated with the investigated *Se*-based solar cell design is demonstrated in details in our previous works [22,23]. As a result, the final formulations of both absorbance and total reflection are basically wavelength dependent and can be given as follows

$$A_i(\lambda) = \frac{\int_V \frac{1}{2} |\vec{E}_y(\vec{r})|^2 \omega \epsilon_0 \epsilon_i''(\lambda) dV}{\int_S \frac{1}{2} \text{Re}\{\vec{E}_y(\vec{r}) \times \vec{H}^*(\vec{r})\} dS} \quad (2)$$

$$R_i(\lambda) = \frac{\int_{port1} (E_{ci} - E_{li}) E_{li}^* dA_1}{\int_{port1} (E_{li} E_{li}^*) dA_1} = \frac{\text{reflected power}}{\text{Incident power}} \quad (3)$$

where A_i and R_i represent absorbance and reflectance of the considered *ZnMgO/Se/Metal/MoO₃/Al* structure, respectively, ϵ_0 denotes the permittivity of the vacuum, while, ϵ_i'' refers to the imaginary component of the complex dielectric constant, \vec{H}^* represents the Magnetic field conjugate, E_{ci} is the electric field on the first port. The parameter E_{li} is the electric pattern at the first port, which is suggested at the top of the investigated *Se*-based solar cell.

It is important to note that the materials, (*ZnMgO*, *Se*, *Au*, *Ti* and *MoO₃*), refractive indexes (n , K) used for estimating both absorbance and reflectance of the analyzed *ZnMgO/Se/Metal/MoO₃/Al* structures are extracted from *SOPRA* database and other experimental works [24–27].

Total absorption efficiency (*TAE*) as an important performance figure of merit, can provide a global insight about the role of the inserted ultrathin *MLs* in improving the *Se*-based solar cell optical behavior. To this extent, this parameter is estimated by means of the following equation

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