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Effect of the n-$MoTe_2$ interfacial layer in cadmium telluride solar cells using SCAPS

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ABSTRACT

The SCAPS-1D simulation package is applied to investigate the possible influences of the n-$MoTe_2$ transition metal dichalcogenide material buffer layer in the CdTe thin film solar cells. The electrical properties and the photovoltaic parameters of the CdTe thin film solar cells, with Molybdenum as a back contact, are addressed. The doping concentration, bandgap energy, and layer thickness of the n-$MoTe_2$ have been varied for this study. It was found that the n-$MoTe_2$ has a remarkable influence on the performance of CdTe thin film solar cells. The efficiency drops from 28.0% to 26.8% as the carrier concentration increases from 1×10^{16} cm^{-3} to 5×10^{16} cm^{-3}, respectively. An optimum efficiency of about 12.7% has been obtained at a bandgap value of 0.95 eV. Finally, the thickness of the $MoTe_2$ layer should be not less than 80 nm to maintain the remarkable overall solar cell performance.

1. Introduction

CdTe is one of the promising candidates with nearly ideal photovoltaic properties. The compound exhibits a relatively high absorption coefficient of $\sim 10^5 cm^{-1}$. They also have congruent evaporation, low cost, and high efficiency reported solar cell [1,2]. CdTe is an II—VI binary compound semiconductor of about 1.5 eV direct band gap matching the optimum range of the solar spectrum for photovoltaic energy conversion. Theoretical works indicate that it is possible to obtain conversion efficiencies of 17% [3]. Conversion efficiencies greater than 15% have already been reported for CdS/CdTe solar cells. One of the key parameters of the solar cell performance is the formation of an ohmic or quasi-ohmic back contact in order to obtain low series resistance for the cell [4]. Therefore, it is believed that the formation of a suitable thin layer is vital for facilitating a quasi-ohmic electrical at the back contact of the solar cell. Previous studies have been reported for the formation of a suitable buffer layer of layered materials [5,6]. For CdTe solar cells the n-$MoTe_2$ may have possible formation as interface between the Mo and CdTe absorber.

$MoTe_2$ belongs to the layered transition metal dichalcogenide materials (TMDCs). These materials have received much attention because of their interesting anisotropy properties originating from their significant 2D structural character. The TMDCs offer a wealth of electronic properties varying from metallic through semiconductors to insulating [7,8]. The materials also possess unique morphology as thin, flexible, high-quality dangling bond free surfaces which are very suitable for thin film epitaxial growth techniques.

The TMDC family crystallizes in a layered structure with a formula MX_2, where M stands for a transition metal and X for a Se, S, or Te chalcogen atom. Single crystals of TMDC are formed by stacks of X–M–X layers, where a sheet of metal atoms is sandwiched between two sheets of chalcogens. Within each layer the atoms are held together by strong covalent-ionic mixed bonds, while the bonding between the layers is a relatively weak Van der Waals type [7,9]. Crystals of such materials show a good cleavage in the direction perpendicular to the layers (*c*–axis). The orientation of this *c*–axis is essential for defining the properties of the solar cell

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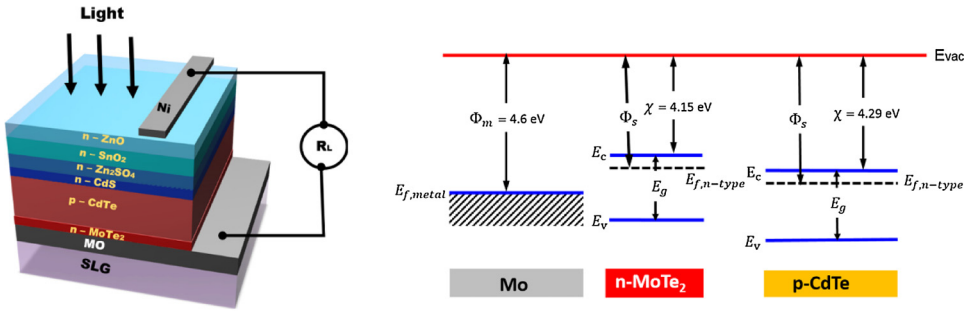

Fig. 1. Left: Schematic diagram of CdTe solar cell using n-$MoTe_2$ TMDC as interfacial layer. Right: Energy band diagrams of Mo, n-$MoTe_2$ and CdTe layers in isolation.

depending on whether the grains are found to be parallel or perpendicular to the *c*-axis [5,7]. In this study, we are concerned with the $MoTe_2$ crystals. This material belongs to group VI with transition metal Mo and chalcogens Te and crystallize in a layered $2H_b$ polytype hexagonal crystal structure. Additionally, the electronic structure of the transition metal Mo in the $MoTe_2$ is $4d^25s^2$ and that of chalcogen Te, which possess higher electron affinity with respect to the transition metal, is s^2p^4. They are semiconductors due to the weak *p-d* interactions. The band structure both experimentally and calculations for the TMDC materials have been investigated by many groups using different approaches and methods [10–12]. Recently, we have presented a comprehensive study on the band structure of some TMDCs using angle resolved photoemission spectroscopy (ARPES) [13].

In this paper, a comprehensive analytical study of the effects of n-type $MoTe_2$ TMDC interfacial layer in between the CdTe absorber layer and the conventional back contact layer Mo, employing the simulation program Solar Cell Capacitance Simulator in one Dimension (SCAPS-1D) numerical modeling, is presented.

2. Simulation and analysis

In this numerical study, SCAPS-1D is used to investigate the effects of n-$MoTe_2$ layer formation in CdTe thin film solar cell. SCAPS is a software developed at University of Gent [14]. It is widely used for the simulation of different types of solar cells, e.g. CIGS and CdTe based solar cells. SCAPS calculates the steady-state band diagram, recombination profile, and carrier transport in one dimension, based on Poisson equation together with hole and electron continuity equations [15]. It has been modeled under an AM 1.5 light spectrum and a 1000 (W/m^2) light intensity.

We report here on the investigation of the effects of n-type $MoTe_2$ formation between Mo back contact and CdTe absorber. Fig. 1(a) depicts the schematic structure of CdTe solar cell with the proposed $MoTe_2$ interfacial layer. Incorporating the various material parameters into SCAPS-1D for all of the analysis aspects, solar cell performance parameters such as open-circuit voltage V_{oc}, short circuit current density Jsc, and fil factor FF as well as the conversion efficiency are investigated. The various material properties used for numerical analysis are collected in Table 1 from Refs. [16–19] and for the interfacial layer from [17,20]. The input values, the absorber thickness and the energy bandgap of $MoTe_2$ layer have been changed from 5 to 200 nm and from 0.8 to 1.1 eV, respectively. The carrier concentration of n-$MoTe_2$ is varied from 5×10^{15} to 5×10^{16} cm^{-3}. For understanding the effects of the $MoTe_2$ interfacial layer on the electrical and photovoltaic properties of CdTe based solar cells, the energy band profile of Mo/$MoTe_2$/CdTe structure is depicted in Fig. 2(b). The interfaces of Mo/$MoTe_2$/CdTe basically depend on the conductivity type of $MoTe_2$. The Mo/$MoTe_2$ metal-semiconductor junction can be either an ohmic or rectifying type, depending on the crucial work function values of the metal and semiconductor, Φ_m and Φ_s, respectively.

Table 1
Material properties applied in the numerical analysis for the CdTe based solar cell at 300 K, as well as for the $MoTe_2$ interfacial layer [16,19].

Parameter	$MoTe_2$	CdTe	CdS	Zn_2SO_4	SnO2	ZnO
Thickness (μm)	0.05 – 0.2	2	0.08	0.1	0.07	0.5
ε_r	13	9.4	9	9	9	9
$\mu_n(cm^2/Vs)$	110	320	350	32	100	320
μ_p (cm^2/Vs)	426	40	50	3	25	40
$N_A(cm^{-3})$	0	10^{19}	0	0	0	0
$N_D(cm^{-3})$	10^{13}–10^{17}	0	10^{19}	10^{17}	10^{17}	10^{18}
$E_g(eV)$	0.8 – 1.1	1.45	2.42	3.35	3.6	3.3
$N_c(cm^{-3})$	3×10^{18}	7.5×10^{17}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}
$N_v(cm^{-3})$	4×10^{16}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
$v_{t-h}(cm/s)$	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
$v_{t-e}(cm/s)$	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
χ (eV)	4.15	4.29	4.5	4.5	4.5	4.45

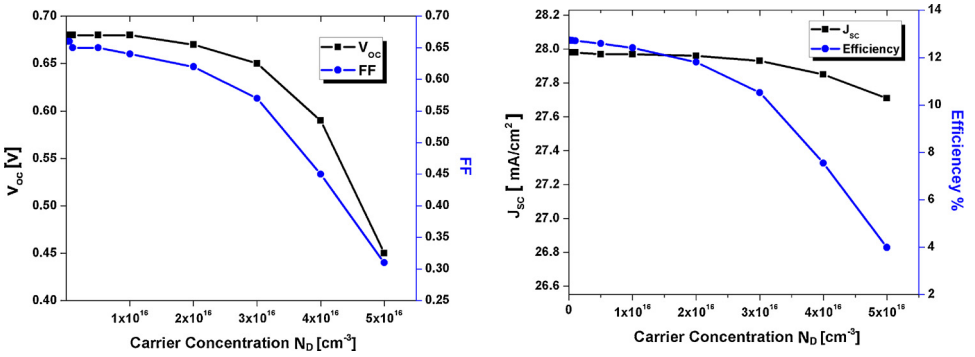

Fig. 2. CdTe performance parameters as a function of n-$MoTe_2$ carrier concentration. Left: short circuit current density J_{sc} and conversion efficiency. Right: fil factor FF and open-circuit voltage V_{oc}.

$MoTe_2$ layer with different type of conductivities is also assumed to have an influence on the equilibrium contact potential (V_o), which forms between Mo/$MoTe_2$ junction because of the dependency of Φ_s to the conductivity type (n or p) and donner and acceptors doping concentration (N_D or N_A). Equilibrium contact potential (V_o) is defined as the difference between the values of metal and semiconductor work function potentials. In metal/ n-type semiconductor junction, the diffusion of electrons from the semiconductor side to the metal side is prevented by this V_o. From the heterojunction point of view n-type $MoTe_2$ forms isotype heterojunction with p-CdTe absorber layer. Additionally, varying the energy bandgap of $MoTe_2$ semiconductor (p-type or n-type) may cause change in the electron affinity. The type of heterojunction is isotype for the semiconductor- semiconductor and of rectifying for the Mo-n-$MoTe_2$ interface.

3. Results and discussion

Fig. 2 shows the solar cell photovoltaic parameters as a function of the carrier concentration (N_D). It can be observed that an increase in the carrier concentration leads to a decrease in the V_{oc}, J_{sc}, FF as well as the conversion efficiency. To explain the obtained results, the interface properties are taken into consideration. From one side, the Mo/n-$MoTe_2$ one, increasing the donor concentration for n-type semiconductor shifts the Fermi level of the semiconductor upwards, i.e., closer to the conduction band, hence the work function decreases. This eventually yields to less ohmic contact at the Mo/n-$MoTe_2$, and the equilibrium contact potential V_o increases. Since the (V_o) is responsible for the inhabitation of the electrons diffusion into metal from n-$MoTe_2$. In contrary, decreasing the doping level resulted in more electrons collection at the back contact Mo side which in turns should increase the conversion efficiency as a result. On the other side, the n-$MoTe_2$/p-CdTe one, increasing the doping level increases the built in potential for the n-$MoTe_2$/p-CdTe. Accordingly, the photogenerated electrons in the vicinity of p-$MoTe_2$/p-CdTe junction will be drifted towards the back contact. In total, increasing the doping level n-$MoTe_2$ reduces the V_{oc} and the efficiency for the solar cell due to electron recombination at the Mo back contact caused by the additional built in potential at n-$MoTe_2$/p-CdTe junction. It is observed that, when the carrier concentration is increased from 1×10^{16} cm^{-3} to 4×10^{16} cm^{-3} the short circuit current density J_{sc} is almost constant of about 28 mA/cm^2, with a slight decrease from 4×10^{16} cm^{-3} to 5×10^{16} cm^{-3}. As per literature, this parameter has been found to be mostly affected by the decrease of the absorber thickness. This is mainly due to the recombination of photogenerated electrons at the back contact [20]. However, in this study, since the absorber thickness is kept constant, no dramatically change in the J_{sc} has been observed. Moreover, solar cell performance parameter V_{oc} observed to decrease by ~30% and the FF by ~50%, i.e. from 0.67 V to 0.47 V and from 0.65 to 0.31 for the V_{oc} and the FF, respectively. A reduction of the V_{oc} will collectively reduce the conversion efficiency of the solar cells. The efficiency has been observed to drop from 28.0% to 26.8% with doping level increasing from 1×10^{16} cm^{-3} to 5×10^{16} cm^{-3} (Fig. 2). The results suggest that increasing the doping level of the n-$MoTe_2$ leads to an efficiency decrease of the performance parameters in this numerical study. It is concluded that the doping level should be in the range of 1×10^{16} cm^{-3} to guarantee a good performance of the solar cell.

In regard to the effect of the bandgap energy on the cell performance due to the added interface n-$MoTe_2$ layer, the band gap has been varied in the range from 0.8 eV to 1.10 eV. Fig. 3 depicts the obtained simulated results of the solar parameters as a function of the band gap. To understand the role of the interfacial $MoTe_2$ on CdTe solar cell device performance, we need to study the band offset at $MoTe_2$/CdTe interface. ΔE_c and ΔE_v are the value of the conduction band offset and the difference in the valance bands. As the bandgap energy increases, possibly due to both the downward shift of E_v as well as the upward shift of E_c. The value of the conduction band offset (ΔE_c) increases, and the value of the valence band offset (ΔE_v) decreases. Therefore, the electrons which were drifted towards n-$MoTe_2$/p-CdTe interface with greater ease, now slightly impeded by the increase of ΔE_c. Additionally, the decrease of ΔE_v will help hole transport causing the impeded holes to go easier. Since the value of ΔE_c at n-$MoTe_2$/CdTe junction is quite low (~0.14 eV) and the value of ΔE_v is quite high (> 0.6 eV), therefore, we suggest that the former effect is greater than the later one, and the major impact will be due to the decrease of ΔE_v. As such, increasing E_g from 0.8 eV to 1.10 eV cause the conversion efficiency to reach an optimum value of 12.8% at band gap of 0.95 eV. The overall cell performance improves up to optimum value of E_g = 0.95 eV then slightly decreases, see Fig. 3. The decrease of the band gap energy of $MoTe_2$ above 0.95 eV suggests that n-$MoTe_2$

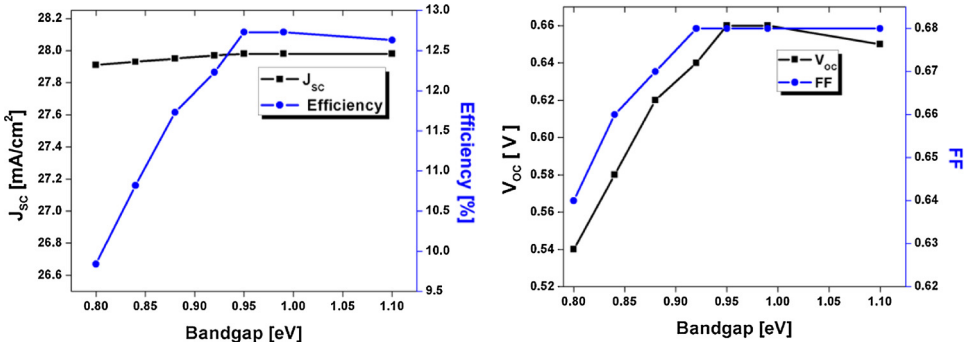

Fig. 3. CdTe performance parameters as a function of n-$MoTe_2$ energy band gap. Left: J_{sc} and conversion efficiency. Right: FF and V_{oc}.

layer acts as a barrier for the holes transport from CdTe toward the back contact, which in turn saturates the cell performance parameters as a result. It can be claimed here that, increasing the band gap will lead to more quasi-ohmic contact and an increase in the overall performance. Similar results have been observed experimentally for the insertion of $MoSe_2$ layer for the CZTS and CIGS based solar cells [21,22].

Furthermore, numerical simulation results as shown in Fig. 4 reveal that when the thickness of the n- $MoTe_2$ layer, with optimized E_g of 0.95 eV, is less than 80 nm, the overall cell performance is low. For example, the V_{oc} decreases from 0.7 V with 80 nm layer thickness and reduces to about 0.37 V at 80 nm layer thickness. This might be attributed to the possibility of creating shunt resistance accompanied with the thinner $MoTe_2$ layer, this can be also observed from the low V_{oc} value. It can be concluded that, $MoTe_2$ layer with thickness less than 80 nm dramatically decreases that the overall cell performance. Hence, based on the numerical simulation outcome from this study, it is very likely that n-type $MoTe_2$ layer with appropriate thickness forms in between Mo layer and p-CdTe layer. Our results agree well with some previous work, experimental investigation addressed that a thickness of $MoSe_2$ interfacial layer is in the range of 100 nm [22]. Finally, it can be considered that the interface layer with thickness plays a vital impact on the overall solar cell performance.

4. Summary

CdTe based solar cell with insertion of interfacial TMDC layered materials, namely n-$MoTe_2$ has been numerically studied, using SCAPS-1D simulation. The simulated results have been analyzed by the study of the energy line band and interface parameters. Reducing the charge carrier concentration of n-$MoTe_2$ resulted in quasi-ohmic contact between the Mo back contact and n-$MoTe_2$ as well as a rectifying contact formation between n-$MoTe_2$ and p-CdTe. It is concluded that the doping level should be in the range of 1×10^{16} cm^{-3} to maintain good performance of the solar cell. The overall conversion efficiency was observed to increase as a function of the band gap and reaches its maximum of ~12.7% at E_g of 0.95 eV. Finally, the thickness of the interfacial layer has been found to be of about 80 nm to maintain a remarkable overall performance of the solar cell.

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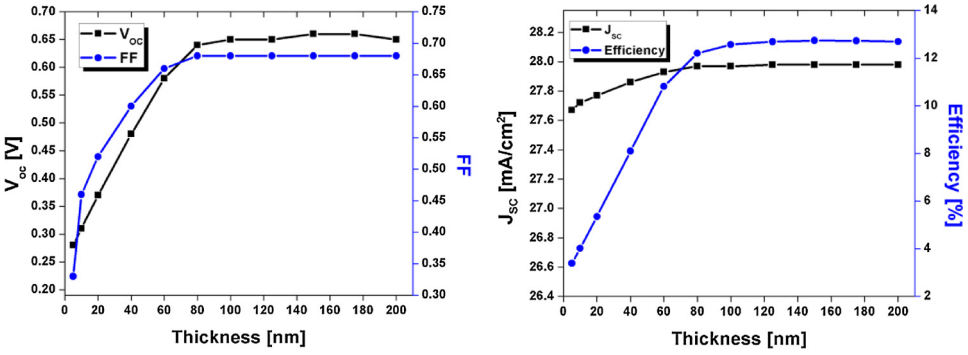

Fig. 4. CdTe performance parameters as a function of n-$MoTe_2$ thickness. Left: J_{sc} and conversion efficiency. Right: V_{oc} and FF.

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