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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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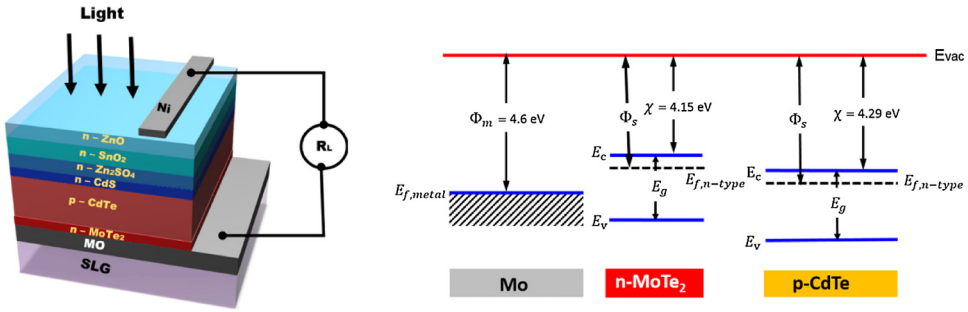

Fig. 1. Left: Schematic diagram of CdTe solar cell using n-$MoTe_2$ TMDC as interfacial layer. Right: Energy band diagrams of Mo, n-$MoTe_2$ and CdTe layers in isolation.

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