Simulation of ZnMgO as the window layer for CdTe Solar Cells

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***Abstract* — CdS has been used as window layer for CdTe solar cells during the last decades of years. New wider band gap (E_g) materials is being found to replace CdS in order to remove blue loss so that short-circuit current (J_{SC}) of CdTe solar cells can be significantly increased. ZnMgO, synthesized by incorporating Mg content into ZnO, is one of the potential candidates. Some researchers have already successfully made high efficiency CdTe solar cells using ZnMgO. In this work, ZnMgO is used as the window layer and systematic computer simulation is finished to investigate the influence of the resistivity (R) of ZnMgO and the conduction band offset (ΔE_C) between ZnMgO layer and CdTe layer on the performance of CdTe solar cells. Simulation results indicate that low resistivity and high doping is needed for ZnMgO and the influence of conduction band offset is quite different when the doping concentration of ZnMgO varies. +0.2eV is an acceptable value for conduction band offset and the ideal Mg content in ZnMgO is around 10%. Finally, a new optimized CdTe solar cell with highest efficiency is designed and a flat band diagram is plotted.**

***Index Terms* — CdTe solar cells, window layer, ZnMgO, resistivity, conduction band offset.**

I. INTRODUCTION

CdTe solar cells are one of the three major branches of the thin film photovoltaic technology. It needs an n-type window layer to form a p-n junction with p-type CdTe layer. CdS has been used as the window layer during the last decades of years. However, with a relatively low band gap, the blue loss will happen that can significantly reduce J_{SC} of CdTe solar cells. The efficiency loss by this blue loss is estimated as 2.3%. [1] Thus, it is helpful to find a new wider band gap material to replace CdS as the window layer in order to improve the efficiency of CdTe solar cells. Actually, the noticeable and dramatic efficiency improvement of CdTe solar cells recently is mainly originated from changing the window layer of CdTe solar cells. Many attempts have been made to find other proper window materials. ZnMgO is one of the potential candidates. Researchers from Colorado University successfully made a CdTe solar cell with efficiency reaching 18.3% by using ZnMgO directly as window layer. [2] However, deep discussion of ZnMgO as window layer is still required for the purpose of making best performance CdTe solar cells.

The first one is the resistivity of ZnMgO. As a window layer, ZnO should not be too resistive and should be highly doped. Otherwise, normal carrier transportation can be impeded, and thus decrease the short-circuit current of CdTe solar cells. On the other hand, window layer also has a function of 'buffer', which means they cannot be too conductive. Otherwise, contents in back contact material, such as Cu, can diffusion into TCO. CdTe solar cells then will be short-circuited and the open-circuit voltage (V_{OC}) of them can be extremely low.

The second one is the conduction band offset between ZnMgO layer and CdTe layer. The band gap of ZnMgO can range from 3.3eV (band gap of ZnO) to 7.8 eV (band gap of bulk MgO) or 6 to 6.5eV (band gap of nanoscale MgO) with the variation of Mg content. [3, 4] The electron affinity (χ) of ZnO is 4.3eV. According to common anion rule, materials with same anions should have very small conduction band offset. This means the change of band gap of ZnMgO will mainly leads to the change of conduction band offset. The conduction band offset has strong influence on the performance of CdTe solar cells. To acquire the highest efficiency CdTe solar cells, a certain range of conduction band offset is highly desired. [5] For the case of ZnMgO, the influence of conduction band offset on the CdTe solar cells still needs to be further investigated. Once the best value of conduction band offset is determined, the Mg content can be calculated from the equation (1). [6]

$$E_g=3.296+2.19x \quad (1)$$

where x is the atomic percent of Mg in the Zn/Mg alloy.

In this paper, SCAPS simulation is employed to find out the influence of resistivity of ZnMgO and conduction band offset on the performance of CdTe solar cells. Brief explanation of the simulation results is provided and a flat band diagram of the highest efficiency CdTe solar cell simulated is plotted.

II. METHOD

SCAPS (a solar cell capacitance simulator) is a one dimension computer program that is commonly applied in the research of solar cell areas. [7] Different kinds of solar cells with different layers including the interfaces between the layers can be built by the program. Then the program numerically solves equations, such as Poisson and continuity equations, for electrons and holes in one dimension to determine the band diagram of the solar cells devices and their response to illumination, voltage bias and temperature. By doing this, the performance of the solar cells can be simulated. Typical examples are J-V, C-V and QE.

A solar cell with the following orders is set up for the simulation. Back contact/ p-type CdTe/ (interface)/ n-type ZnMgO/ TCO / front contact. All the parameters in this simulation are shown in TABLE I. Part of the parameters are achieved from other publications. [8, 9]

According to Equation (2), when the mobility (μ) of the ZnMgO is fixed, the resistivity of ZnMgO is only determined by the doping concentration (n) of it.

$$R = \frac{1}{\mu q n} \quad (2)$$

Thus, to simulate the influence of the resistivity of ZnMgO on the performance of CdTe solar cells, the simulation variable is the doping concentration of ZnMgO, while the other parameters are kept the same.

As mentioned above, the common anion rule tells us that materials with the same anions should have very small valence band offset. But it is not absolutely true in every case. In this paper, we assume by increasing the band gap of ZnMgO, 80% percent of the increment will go to conduction band, while the other 20% will go to valence band. For example, when the band gap of ZnMgO increases 0.1eV, the conduction band offset will increase 0.08eV and valence band offset will increase 0.02eV. From Anderson's rule, the conduction band offset is related to the electron affinity that forms the heterojunction. Accordingly, to simulate the influence of the conduction band offset between ZnMgO layer and CdTe layer on the performance of CdTe solar cells under the conditions of different doping concentration of ZnMgO, the variables of the simulation are the band gap of ZnMgO and its related conduction band offset. The other parameters are kept the same.

Once the ideal band gap of ZnMgO is determined, the Mg content for ZnMgO to yield highest efficiency CdTe solar cell will be calculated and the flat band diagram of the highest efficiency CdTe solar cell simulated is plotted.

III. RESULTS

A. The influence of resistivity of ZnMgO on the performance of CdTe solar cells

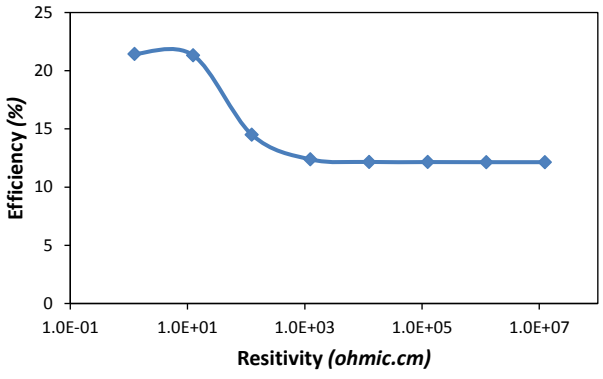
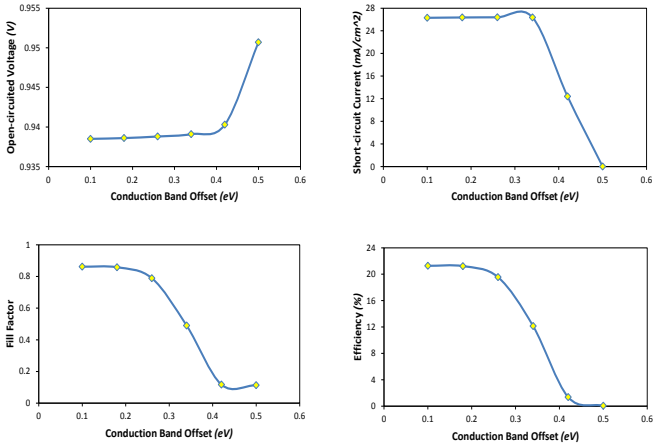


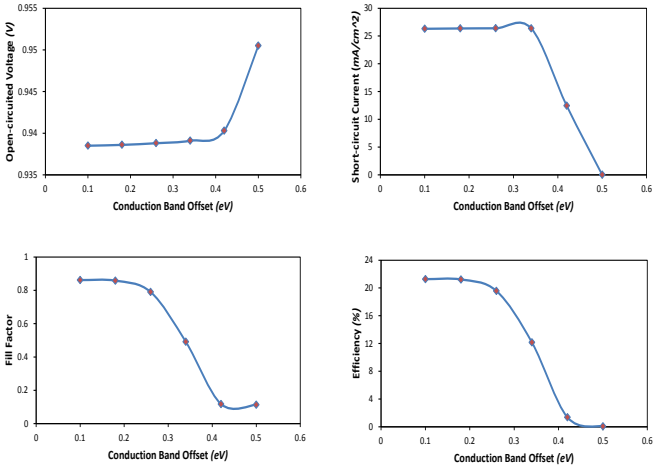
Fig.1. The efficiency of CdTe solar cells as a function of the resistivity of ZnMgO

Figure 1 shows the efficiency of CdTe solar cells in terms with the doping concentration of ZnMgO. Information from the figure indicates that the doping concentration of ZnMgO should be as high as possible. However, this information could be wrong since the ZnMgO layer may also play a role of buffer in CdTe solar cells. It can help prevent the immigration of some harmful elements, for example Cu, into the front contact. If the doping concentration of ZnMgO is too high, the undesired immigration of the harmful elements maybe significantly enhanced. This kind of immigration will make the CdTe solar cells short-circuited, which should be avoided. Since SCAPS is a one-dimension simulation program, the function of a buffer layer cannot be simulated. This means the information achieved from Figure 1 may be overthrown and the optimal doping concentration of ZnMgO should be further investigated by experiments.

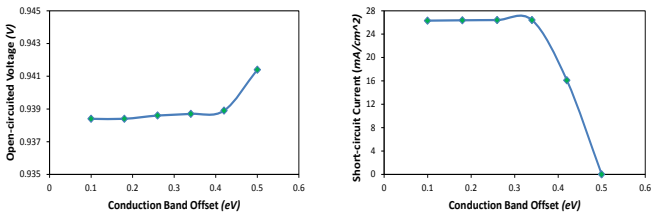
B. The influence of the conduction band offset between ZnMgO layer and CdTe layer on the performance of CdTe solar cells



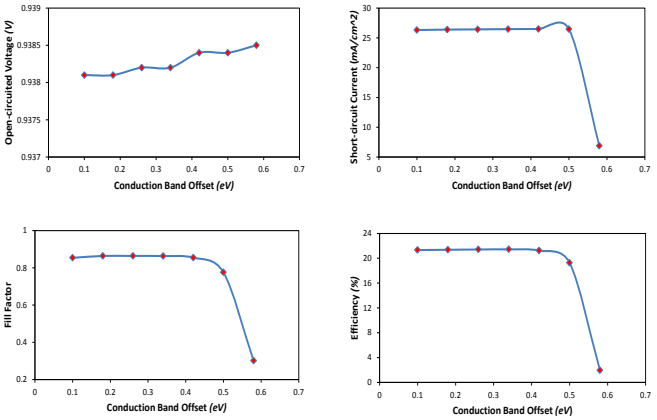
(a)



(b)



(c)



(d)

Fig.2. The performance of CdTe solar cell as a function of conduction band offset between ZnMgO layer and CdTe layer. (a) when the doping concentration of ZnMgO is 10^{11}cm^{-3}, (b) when the doping concentration of ZnMgO is 10^{14} cm^{-3}, (c) when the doping concentration of ZnMgO is 10^{16} cm^{-3}, (d) when the doping concentration of ZnMgO is 10^{18} cm^{-3}.

Figure 2 shows the influence of the conduction band offset on the performance of CdTe solar cells with the doping concentration of ZnMgO shifted.

The open-circuit voltage of CdTe solar cells increase slightly together with the conduction band offset. A proper explanation is the surface recombination rate is decreased when the conduction band offset is increased. This leads to the increase of carrier lifetime and further the decrease of dark current. Then, from either Shockley's model or Shockley-Read- Hall, the open-circuit voltage is increased because it is inverse proportional with the carrier lifetime. In addition, the increase of conduction band offset can also enhance the upper limit of the open-circuit voltage, which is the built-in voltage of CdTe solar cells, from Equation (3).

$$V_{OC} \leq V_{bi} = 1/q\ (E_{gp} + \Delta E_C - \Delta E_n - \Delta E_p) \quad (3)$$

The short-circuit current and fill factor of CdTe solar cells decrease dramatically when the conduction band offset is too big. The reason is that a positive conduction band offset acts as a 'spike', which can prevent the movement of the photo-generated electrons from CdTe layer to ZnMgO layer. Then the short-circuit current will be subsequently reduced. However, if the positive conduction band offset is not too big, the electrons can use the thermal energy to climb through the 'spike' barrier and the solar cell can still work well.

It is also found that at higher doping concentration of ZnMgO, the threshold value of conduction band offset for short-circuit current to decrease is also higher. A possible explanation is a higher doping concentration of ZnMgO will decrease the value of ΔE_n, which means the the barrier the electrons has to climb through can be decreased a little bit.

The highest efficiencies of CdTe solar cells are obtained with the conduction band offsets of 0.1eV, 0.1eV, 0.18eV and 0.34eV for ZnMgO doping concentration of 10^{11} cm^{-3}, 10^{14} cm^{-3}, 10^{16} cm^{-3} and 10^{18} cm^{-3}, respectively. It looks that +0.2eV for the conduction band offset is always in the range of best performance CdTe solar cell no matter what the doping concentration of ZnMgO is. So the ideal Mg content for ZnMgO should be around 10% from Equation (1).

C. The flat band diagram of the simulated highest efficiency CdTe solar cell

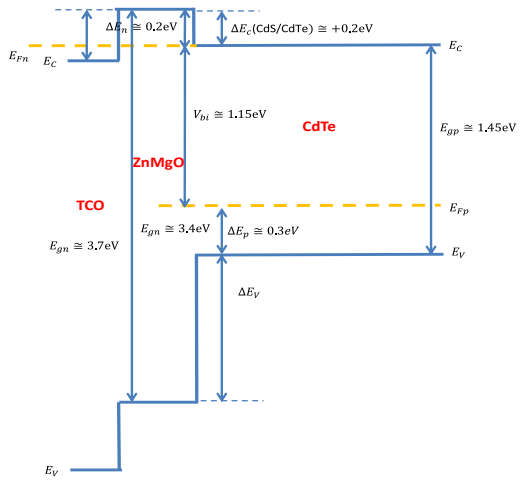


Fig.3. The flat band diagram of the simulated highest efficiency CdTe solar cell.

Figure 3 depicts the flat band diagram of the simulated highest efficiency CdTe solar cell. The doping concentration for the ZMO is 10^{18} cm^{-3}. The Mg content for ZnMgO is 10%, which forms a +0.2eV conduction band offset between CdTe layer and ZnMgO layer.

IV. CONCLUSION

By increasing doping concentration to decrease resistivity of ZnMgO layer, simulation results indicates that the efficiency of CdTe solar cells improves and starts to reach the highest point when doping concentration is 10^{18} cm^{-3}. But this does not mean that higher doping concentration and lower

resistivity of ZnMgO is desired. The reason is that SCAPS is a one-dimension simulation software and probably cannot reflect the role of ZnMgO as a buffer. The influence of conduction band offset between ZnMgO layer and CdTe layer is quite different when the doping concentration of ZnMgO varies. But +0.2eV is a value that is always in the range of best performance CdTe solar cells whenever the doping concentration of ZnMgO is. The ideal Mg content in ZnMgO is around 10%. Finally, a flat band diagram of the simulated highest efficiency CdTe solar cell is provided when the doping concentration of ZnMgO is 10^{18} cm^{-3} and the conduction band offset is +0.2eV.

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TABLE I

THE PARAMETERS OF THE SIMULATED SOLAR CELL

Layer	TCO	ZnMgO	Interface	p-CdTe
Thickness [nm]	500	70	-	2500
Band Gap [eV]	3.7	3.3-3.8	-	1.5
Electron Affinity [eV]	4.5	4.3-3.9	-	4.4
Relative Dielectric Permittivity	10	9	-	9.4
Density States of Conduction Band [cm^{-3}]	2.2×10^{18}	2.2×10^{18}	-	8.0×10^{17}
Density States of Valence Band [cm^{-3}]	1.8×10^{19}	1.8×10^{19}	-	1.8×10^{19}
Electron Mobility [cm^2/V.s]	32	5	-	320
Hall Mobility [cm^2/V.s]	30	1	-	40
Donor Concentration [cm^{-3}]	1.0×10^{19}	$1.0\times10^{11\text{-}18}$	-	-
Acceptor Concentration [cm^{-3}]	-	-	-	1.0×10^{15}
Dopant energy level [eV]	-	-	-	0.255
Defect Type	SA*	SD*	N*	SD*
Electron Cross Section [cm^{-2}]	1.0×10^{-15}	1.0×10^{-12}	1.0×10^{-15}	1.0×10^{-13}
Hole Cross Section [cm^{-2}]	1.0×10^{-12}	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-15}
Defect Concentration [cm^{-2}]	1.0×10^{16}	1.0×10^{18}	1.0×10^{13}	2.0×10^{13}
Defect energy level [eV]	2.0	1.65	0.6	0.585

* SA = single acceptor, N = Neutral, SD = single donor