ELECTRICAL MODELING OF THE BUFFER LAYER FOR A Cu_2O/ZnO SOLAR CELL USING SILVACO ATLAS

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A numerical analysis of the ZnO buffer layer based on physical modeling in SILVACO Atlas has been carried out for a Cu_2O/ZnO subcell in a Si-based tandem heterojunction solar cell design, in order to evaluate and improve the metal-oxide subcell performance. The influence of the thickness and electronic parameters of the buffer layer on the electrical performance of the Cu_2O/ZnO subcell was investigated. A study for the optimum buffer layer electron affinity has been made to find the most suitable candidate materials. This leads to a conclusion that the ZnO buffer layer could be replaced with a theoretically better Ta_2O_5, β-Ga_2O_3 or a compound zinc oxide buffer layer.

Keywords: solar cell, zinc oxide, buffer layer, cuprous oxide

1. Introduction

Semiconducting metal oxides such as ZnO and Cu_2O have competitive production costs while possessing a high optical absorption and chemical stability and are promising candidate materials for implementation in a Si-based tandem heterojunction solar cell (STHSC). Currently, the highest conversion efficiency for a ZnO/Cu2O heterojunction is about 8% [1], with the potential to reach 14% as reported by Takiguchi [2] and a known theoretical maximum efficiency of 19-20% [3]. The purpose of this paper is to evaluate and optimize the ZnO buffer layer in the metal-oxide subcell. The buffer layer used in the cell is the focus in the current step of the subcell development and this simulation due to its importance in the overall cell design. The buffer material needs to have the proper

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band alignment in the structure, to be used with the Cu_2O layer in a heterojunction. The band alignment takes into account the discontinuities in the valence band maximum energy and the conduction band minimum energy which is in focus here. The alignment of the conduction band, referred to as conduction band offset is one of the important reasons of low open circuit voltages (Voc) [4]. Choosing the right material that suits the low electron affinity of the Cu_2O and has convenient band alignment, would increase the voltages and efficiency of the cells.

2. Materials and Method

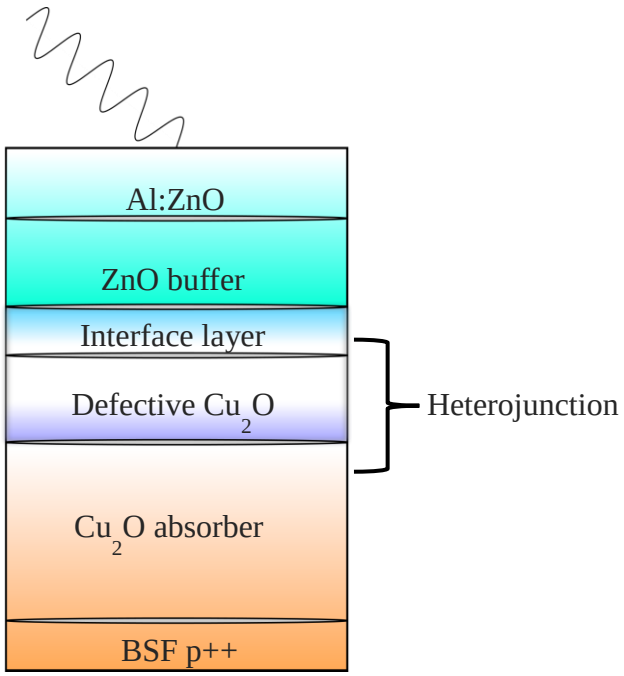

Fig. 1. Schematic of the Cu_2O/Al:ZnO subcell (as implemented by Takiguchi et al.[2])

Simulation of a Cu_2O/Al:ZnO subcell has been done using Silvaco Atlas. The schematic of the Cu_2O/Al:ZnO subcell is shown in Fig. 1. We have calculated the cell short circuit current density, open circuit voltage, power conversion efficiency and external quantum efficiency curves varying key parameters of the ZnO buffer layer, such as layer thickness and electron affinity, in order to improve the current buffer layer and to identify the alternative optimum material for the Cu_2O-based heterojunction subcell. Buffer layer input data are implemented according to Takiguchi's article [2]. We started with 3.65 eV electron affinity and varied the buffer layer thickness up to 0.2 μm and then varied the electron affinity from around 2.5 eV to 5 eV, which would include materials such as Ga_2O_3, Ta_2O_5,

Zn(O,S) and $Zn_{1-x}Ge_xO$. These materials have favorable electron affinity and CBO (conduction band offset) with cuprous oxide, or can be manipulated via compound ratios for proper band alignment [1], [4], [5], [6].

3. Results and Discussion

In Fig. 2, the influence of the buffer layer thickness on the overall cell performance is shown, suggesting an optimum thickness in the range from 0.05 to 0.1 µm while taking into account buffer electron affinity of 3.65 eV.

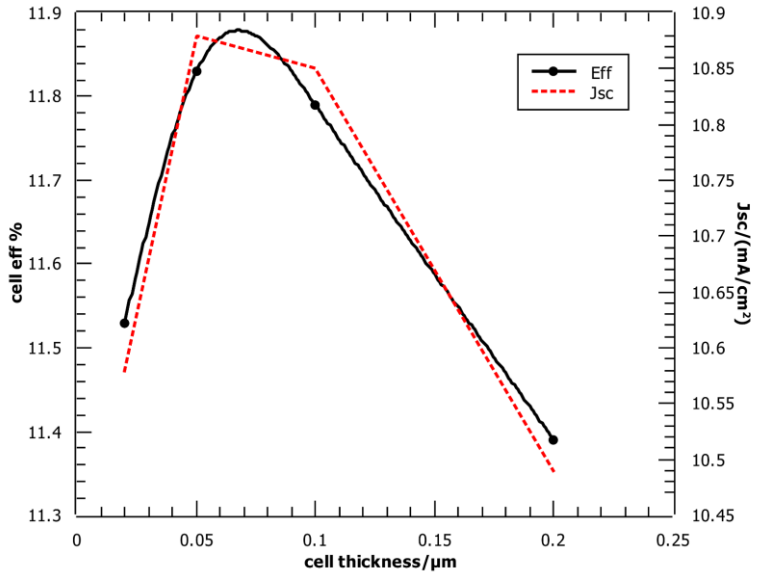

Fig. 2. J_{SC} and power conversion efficiency dependence on the buffer layer thickness

Fig. 3 shows cell open circuit voltage and power conversion efficiency for various electron affinities of the buffer layer. A good performance can be seen in the range from 3.4 eV to 3.7 eV. Fig. 4 shows the external quantum efficiency (EQE) curve for the subcell, for different electron affinities of the buffer layer. The EQE curves suggest that the optimum interval for the electron affinity for the buffer layer is in the range from 3.2 eV to 3.65 eV. In this range, the EQE reaches over 80% in the 360-560 nm wavelength range.

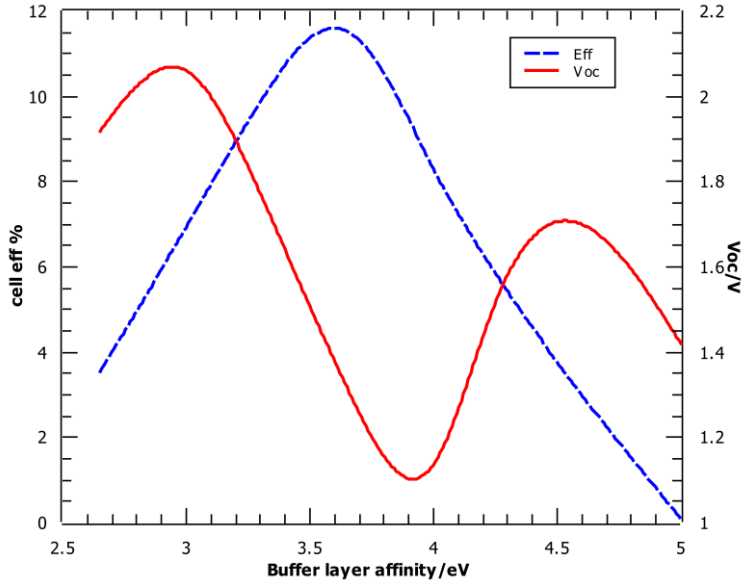

Fig. 3. Voc and cell efficiency dependences on the electron affinity of the buffer layer

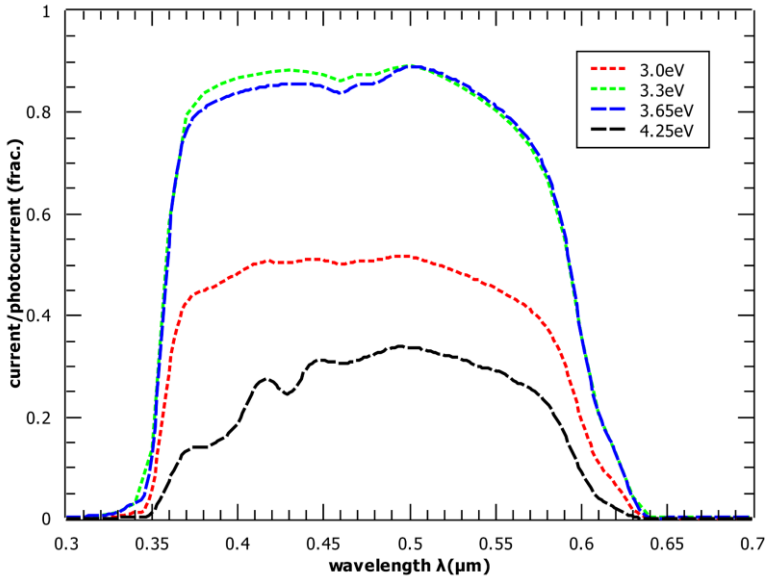

Fig. 4. EQE for different electron affinities for the buffer layer

Comparing our results, it was observed that the current buffer layer (3.65 eV E_{EA}) thickness is optimal in the range from 0.05 μm to 0.1 μm. When results were compared with the key parameters of materials found in literature we saw that the electron affinity is optimal in the range from 3.2 eV to 3.7 eV. Suitable

materials around these values are based on β-Ga_2O_3, Ta_2O_5, Zn(O,S) and $Zn_{1-x}Ge_xO$.

Energy band alignment has been properly discussed in literature [7], [8] and the effect of the CBO on the open circuit voltage has been analyzed by Brandt et al. [4]. Therefore, it is known that for Cu_2O devices, large conduction band offsets mean lower open circuit voltages. A conduction band offset optimized for peak open circuit voltage is around ±0.2 eV [9]. Layer deposition method has a great influence on the energy band alignment at the interface. However, band alignment can be manipulated at metal-oxide heterojunctions with intrinsic defects and impurities for the constituents, because this way the Fermi level position can be controlled and therefore reduce the conduction band offset. That being said, the multi-component zinc oxide, where we have tunable conduction bands, can control the compound ratios and defects properties are suitable for Cu_2O-based heterojunctions. Among these, Zn(O,S) [6] and $Zn_{1-x}Ge_xO$ [1] have been investigated and confirmed as candidate materials for buffer layer implementation in a metal-oxide solar cell. Ga_2O_3 is another good option here, because it offers a good electronic alignment with a band offset around 0.38 eV [4] and a smaller electron affinity than ZnO. Ga_2O_3 also yields good efficiencies in literature studies and experiments [10], [11]. Ta_2O_5 also has favorable conduction band offset, and can be manufactured at low temperature [5]. Its electron affinity is closer to the cuprous oxide [12] and therefore another good potential candidate for the buffer layer in a Cu_2O-based heterojunction solar cell. These materials are in focus for ongoing experimental studies in order to optimize the Cu_2O-based [13] heterojunction subcell for the silicon tandem implementation.

4. Conclusions

In this work, SILVACO Atlas was adopted to investigate the influence of the thickness and electron affinity of the buffer layer on the electrical performance of a ZnO/Cu_2O subcell. A ZnO buffer thickness below 0.1 micrometers is optimal and a buffer layer with electron affinity in the range from 3.2 eV to 3.7 eV is recommended for peak performance of the Cu_2O-based heterojunction subcell.
Suitable candidate materials for the optimum buffer layer are Ta_2O_5, β-Ga_2O_3, Zn(O,S) and $Zn_{1-x}Ge_xO$, which have a closer electron affinity to the cuprous oxide and benefit from convenient band alignment, and so would theoretically, provide a better performance than the original ZnO layer. Further experimental work is required for such materials in order to find the best candidate.

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