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Numerical modeling baseline for high efficiency (Cu_2FeSnS_4) CFTS based thin film kesterite solar cell

Yousaf Hameed Khattak[a,b,*], Faisal Baig[a,b], Shafi Ullah[a], Bernabé Marí[a], Saira Beg[c], Hanif Ullah[b]

[a] Escuela de Ingeniería de Diseño, Departamento de Física Aplicada, Universitat Politécnica de Valencia, Camí de Vera, Spain
[b] Department of Electrical Engineering, Federal Urdu University of Arts, Science and Technology, Islamabad, Pakistan
[c] Department of Computer Science, COMSATS Institute of Information Technology, Islamabad, Pakistan

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ABSTRACT

Cu_2FeSnS_4 (CFTS) is auspicious nontoxic and earth abundant semiconductor compound having kesterite symmetrical structure. It is an attractive and suitable material for the fabrication of low cost, high efficiency and sustainable thin film photovoltaic cell. CFTS based kesterite photovoltaic cell device modeling was performed in this work. The influence of device parameters such as the thickness, acceptor and donor carrier concentration densities of absorber and electron transport layer (ETL), effect of back contact metal work function and the temperature effect on the performance of CFTS based kesterite photovoltaic cell is analyzed by using one dimensional solar cell capacitance simulator (SCAPS) software. In this work, promising optimized results had been achieved with the conversion efficiency of 19.97%, fill factor (FF) 85.94%, short-circuit current (J_{sc}) 23.37 mA/cm^2 and open circuit voltage (V_{oc}) 0.995 V. The above results will give imperative baselines and feasible directions for the fabrication of higher efficiency CFTS based photovoltaic cell.

1. Introduction

Thin film technology is the one of the most cost effective and efficient technology for the manufacturing of photovoltaic cells and it is an excellent subject of intense research in photovoltaic industry. Thin films are very suitable for low and large scale photovoltaic cell applications. To fulfill the consumer demand and for the generation of electricity, the high-power conversion efficiency solar cell without degradation of materials and economical photovoltaic cells are fabricated [1]. Silicon based photovoltaic cells dominated the market from many years and due to intensification in manufacturing capabilities thin film photovoltaic cells are gaining significance [2]. For the manufacturing and production of silicon based thin film solar cell, different major deposition techniques like sputtering, thermal evaporation, molecular beam epitaxy, e-beam evaporation, close space sublimation, and metal organic chemical vapor deposition techniques are attempted [3]. So, cost of the material, technology and energy consumption used by these sophisticated fabrication techniques makes the solar cell panel costly [4]. *CdTe*, *CIGS* ($CuIn_{1-x}Ga_xSe_2$) and related alloy based thin-film chalcopyrite photovoltaic cells materials are commercially used for the fabrication of thin film photovoltaic devices because of high conversion efficiency, excellent electrical as well as optical properties [5] and also these types of devices have high absorption coefficient [6,7]. The toxic materials restrict

* Corresponding author at: Department of Electrical Engineering, Federal Urdu University of Arts, Science and Technology, Islamabad, Pakistan.
E-mail addresses: yousaf.hameedk@gmail.com, yousaf.hameed@fuuastisb.edu.pk (Y.H. Khattak).

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the further development of these types of cells and the rare materials like Indium and Gallium used for the fabrication of cell also increase the fabrication cost [5]. So, the commercial production of *CIGS* based photovoltaic cell is limited.

Non-toxic earth abundant materials having kesterite symmetrical structure like *CZTS* (Cu_2ZnSnS_4), *CZTSe* ($Cu_2ZnSnSe_4$), [8–12] *CFTS* (Cu_2FeSnS_4), *CFTSe* ($Cu_2FeSnSe_4$) and their alloys are emerging as the most auspicious replacement for the chalcopyrite absorbers (*CIGS*, *CIGSe*) [13–15]. The growing attention towards these quaternary compounds for photovoltaic cells production is due to their potential [16–19]. Among these quaternary compounds, *CFTS* is one of the most auspicious compound for an effective light absorber material due to its suitable optical band gap of 1.2–1.5 eV [20–24] and large absorption coefficient $\alpha > 10^4 cm^{-1}$ [18,25–29]. Power conversion efficiency of about 0.29% for *CFTS* based solar cell is presented in [30]. In [26], the reported conversion efficiency is 2.73%.

Numerical modeling or numerical analysis is an essential tool for the better understanding of device working parameters. Numerical analysis can play a significant role in manufacturing and fabrication of an efficient photovoltaic device. Numerical analysis of the kesterite based *FTO*/TiO_2/*CFTS*/*back contact* photovoltaic cell is proposed in this work. In our simulations, thickness of absorber layer (*CFTS*) varies from 1 μm to 4 μm and the bandgap energy is 1.3eV. The band gap of electron transport layer is larger than that of absorber layer; hence, maximum photons are absorbed in *CFTS*, which will increase the overall conversion efficiency of photovoltaic cell. The proposed results will give a valuable baseline for the design of high performance *CFTS* based kesterite solar cells.

2. Solar cell design

Fig. 1 shows our proposed photovoltaic cell structure *FTO*/TiO_2/*CFTS*/*Mo*, which comprises back contact layer *Mo*, absorber layer *CFTS*, electron transport layer TiO_2 and window layer *FTO*. We have investigated the influence of parameters like temperature variations, absorber layer dopant concentration and thickness, electron transport layer dopant concentration and thickness, as well as compensation ratio and illumination power of the sun, on the performance of our photovoltaic cell model. For optimum values of parameters (absorber layer thickness 4μm and acceptor carrier concentration $3 \times 10^{18}\ cm^{-3}$), we found a conversion efficiency of 19.97%.

3. Numerical modeling and material parameters

The simulation software that can be used for the numerical modeling of photovoltaic cell must be able to solve the semiconductor basic equations like the continuity equation for holes and electrons and the poisson's equation relating the charge to the electrostatic potential. The charge carrier transport equation and the basic equations are well explained in simya O.K.et al [31]. We have used one dimensional Solar Cell Capacitance Simulator (SCAP-1D) software developed at the University of Gent, Belgium, to simulate our proposed model of photovoltaic cell. That software is designed for simulations and helps for analysis of J–V characteristics curve, ac characteristics (C-V and C-f), spectral response(QE) of a device, power conversion efficiency (PCE), fill factor (FF), short-circuit current (J_{sc}), open circuit voltage (V_{oc}) used, energy bands of materials used in solar cell and concentration of different material used by solving the semiconductor basic equations, the hole and electron continuity equation and the Poissons equations.

The measure of a photovoltaic cell quality is Fill Factor (*FF*), which is derived by equating the maximum power (P_{max}) to the theoretical power (P_t). Where power (P_t) would be output at both the short circuit current (J_{sc}) and open circuit voltage (V_{oc}) as given in Eq. (1).

$$FF = \frac{P_{\max}}{P_t} = \frac{V_{\max} I_{\max}}{V_{OC} J_{SC}} \tag{1}$$

The product of P_t and *FF*, divided by the energy input from the sun is the power conversion efficiency (*PCE*) mathematically expressed in Eq. (2).

$$PCE = \frac{V_{OC} J_{SC} FF}{P_{in}} \tag{2}$$

The parameters used in SCAPS software for numerical analysis are absorber layer thickness, electron-hole mobility, intrinsic carrier concentration, electron affinity, band gap and doping density. For buffer and window layer similar parameters

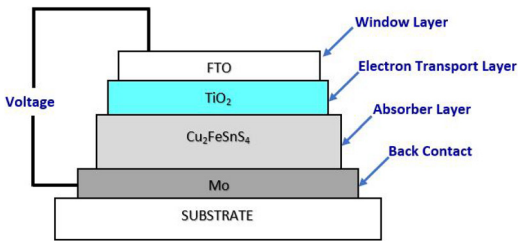

Fig. 1. Block diagram of CFTS solar cell.