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OPTICAL MODELING AND SIMULATION OF TANDEM METAL OXIDE SOLAR CELLS

Florin Drăgan[1], Ørnulf Nordseth[2], Laurențiu Fara[1, 3,*], Constantin Dumitru[1], Dan Crăciunescu[1], Vlad Muscurel[1], Paul Sterian[1, 3]

[1] *University "Politehnica" of Bucharest, Spl. Independentei 313, RO-060042, Bucharest, Romania*

[2] *Institute for Energy Technology, Instituttveien 18, NO-2007 Kjeller, Norway*

[3] *Academy of Romanian Scientists, Spl. Independentei 54, RO-030167, Bucharest, Romania*

[*] *Corresponding author: lfara@renerg.pub.ro*

Article Info	Abstract
Received: 02.03.2018 *Accepted: 15.06.2018* **Keywords:** tandem solar cells, metal oxides, cuprous oxide, zinc oxide, optical modeling, ray tracing, transfer matrix, absorber layer, buffer layer.	An investigation of silicon-based tandem solar cells incorporating Al-doped ZnO (AZO) and Cu_2O metal oxides, via two of the most efficient methods of optical modeling, specifically ray tracing and transfer matrix algorithms, was performed. The simulations were conducted based on specialized software, namely Silvaco Atlas and MATLAB, as well as on OPAL2 simulation platform. The optical analysis involved the calculation of the spectral curves for reflectance, absorptance and transmittance for different thicknesses of the thin film layers constituting the cell. It was established the optimum thickness of the AZO layer based on the minimum reflectance and maximum transmittance. Moreover, several materials were investigated in order to determine the optimum buffer layer for the tandem solar cell, based on optical modeling. The optical parameters of the ZnO/Cu_2O top subcell were optimized, in order to achieve the highest conversion efficiency of such heterojunction solar cell.

1. Introduction. State of the art

Progress in the design of thin film solar cells has accelerated the development of tandem solar cells based on crystalline silicon (c-Si) that yield better conversion efficiencies compared to the c-Si single-junction implementation. Such improvements are required in order to ensure competitiveness versus conventional energy sources [1, 2]. Recently, tandem solar cells have been implemented on III-V type semiconductors, monocrystalline, polycrystalline, and amorphous silicon, dye sensitized solar cells, and quantum dot solar cells. The commercial manufacturing of silicon based tandem heterojunction solar cells (STHSC) with high efficiency and low cost has not been achieved yet. A promising material for a STHSC implementation is cuprous oxide (Cu_2O) [3, 4, 5]. This semiconducting metal oxide has a high optical absorption, is non-toxic, and has the potential for low production cost [6, 7, 8]. The theoretical limit of the conversion efficiency for a solar cell based on Cu_2O is close to 20% under one sun illumination. However, the literature reports that the highest conversion efficiency achieved experimentally is 8.1% for a ZnO/Cu_2O solar cell based on thermally oxidized copper sheets, suggesting that further research of Cu_2O-based solar cells is still needed in order to optimize them for photovoltaic applications.

Figure 1 shows a schematic design of a STHSC, that combines a conventional crystalline silicon bottom subcell with a ZnO/Cu_2O top subcell in a mechanical stack of independently connected cells, i.e . a four-terminal configuration. The high band gap of Cu_2O (E_g = 2.1 eV), which is approximately 1 eV higher than that of crystalline silicon (E_g = 1.13 eV), would yield a less efficient low-cost two-terminal tandem configuration. A four-terminal configuration allows for accessing a wider range of material combinations compared to a two-terminal configuration since there is a constraint on current matching for the two subcells [1, 9].

For the top subcell, a heterojunction between cuprous oxide and a buffer layer (n-type) is being used. Numerical modeling shows that an optimal material implementation for the buffer layer is very important for the electronic and optical performance of the heterojunction [10].

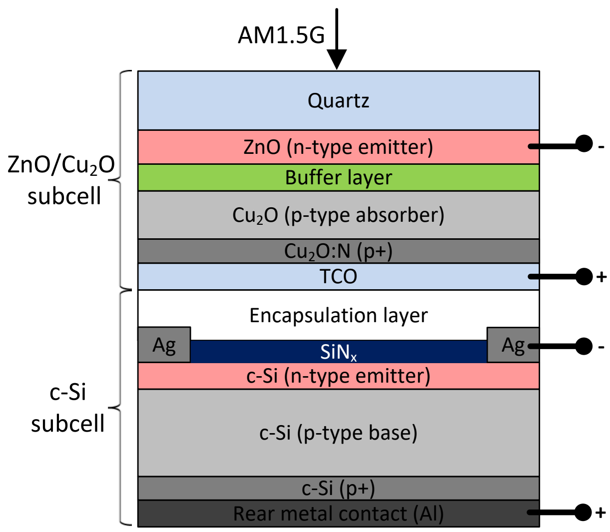


Fig. 1. Schematic of the four-terminal tandem metal oxide solar cell [9]

This paper presents a review of different optical modeling and numerical simulation studies of the STHSC, recently published by the authors. The optical analysis involves ray tracing method to calculate the spectral curves for reflectance, absorptance, and transmittance for different thicknesses of the thin film layers of the ZnO/Cu_2O subcell. Such approach can provide useful information for the layer optimization, in order to ensure efficient light management in the solar cell.

2. Methods of optical modeling for advanced solar cells

2.1 Main methods for optical modeling

Using Technology Computer-Aided Design (TCAD) simulation software, such as Silvaco Atlas [11], the propagation of light can be described by any of the four physical models or several user defined approaches. The physical models for light propagation include the following:

• Ray tracing (RT) is a general method of resolving 2D and 3D non-planar geometries but ignores coherence and diffraction effects.

• The transfer matrix method (TM) is a 1D method that includes interference effects. This method is recommended for large area devices such as thin film solar cells.

• The beam propagation method (BP) is a general 2D method that includes diffraction effects at an increased computational expense.

• Finite difference time domain (FDTD) is the most general 2D and 3D method and accounts for both diffraction and coherence by direct solution of Maxwell's equations. This is the most computationally expensive approach.

This review article is based only on two methods, respectively ray tracing (RT) and transfer matrix (TM).

2.2. Ray tracing method

Optoelectronic device simulation is split into two distinct models that are calculated simultaneously at each DC bias point or transient timestep:

1. Optical ray trace using real component of refractive index to calculate the optical intensity at each grid point;

2. Absorption or photogeneration model using the imaginary component of refractive index to calculate a new carrier concentration at each grid point.

Ray tracing in 2D

An incident optical beam is modeled as a collimated source. As shown in Figure 2a, the illumination window is "clipped" against the device domain so that none of the beam bypasses the device. The beam is automatically split into a series of rays so that the sum of the rays covers the entire width of the illumination window. When the beam is split, the software automatically resolves discontinuities along the region boundaries of the device.

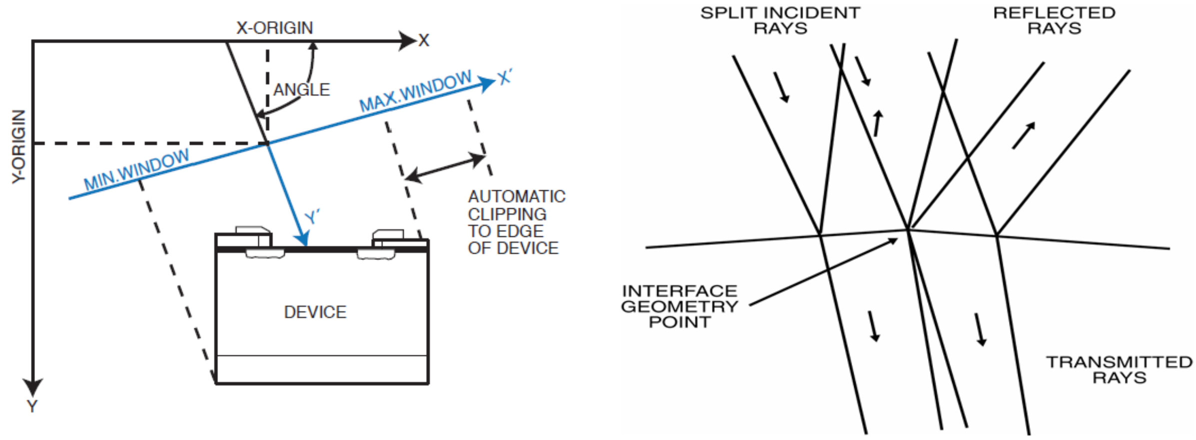


Fig. 2. a) Optical beam geometry; b) Reflected and transmitted rays [11].

Rays are also split at interfaces between regions into a transmitted ray and a reflected ray. Figure 2b illustrates the difference between rays that are split to resolve the geometry and transmitted / reflected rays split at a region interfaces.

Ray tracing in 3D

In 3D, the algorithm doesn't automatically split rays to resolve topological features of the device. The 3D source geometry is very similar to the geometry shown in Figure 2a. In 3D, the source origin is specified by three coordinates for the origin of beam: X,Y, and Z. Unlike Figure 2a, there are two angles that describe the direction of propagation. As can be seen in Figure 3, the angle PHI describes is the angle or propagation with respect to the XZ plane. The angle THETA describes the angle of rotation specified about the Y axis.

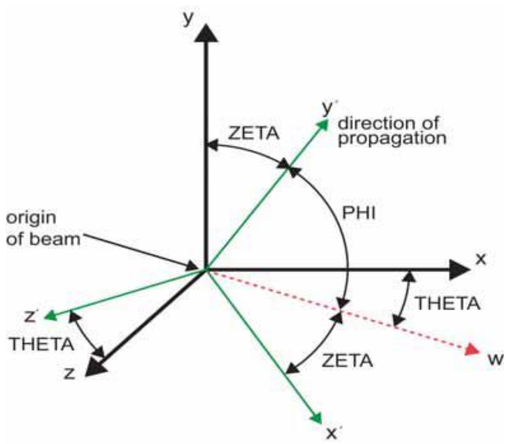


Fig. 3. Propagation in 3D [11].

2.3. Transfer matrix method

The Transfer Matrix (TM) method allows for a fast and accurate way to simulate electromagnetic wave propagation through a layered medium. In the matrix theory, the characteristic matrix and the transfer matrix descriptions are commonly used [11].

The structure of a multilayer stack completely determines its characteristic matrix. The transfer matrix also contains information about the media on both sides of the layer stack. The characteristic matrix approach is considered to be more general and can be expanded to include graded interfaces, in which instance, the transfer matrix method is inappropriate to implement.

The characteristic matrix of a multilayer is basically a product of corresponding single layer matrices. If m is the number of layers, then the field at the first ($z=z_0$) and the last ($z=z_m$) boundaries are related as seen in the equation below:

$$\begin{bmatrix} E(Z_0) \\ H(Z_0) \end{bmatrix} = M_1, M_2 \dots M_m \begin{bmatrix} E(Z_m) \\ H(Z_m) \end{bmatrix}, M_i = \begin{bmatrix} \cos\varphi_i & j\sin\varphi_i / Y_i \\ jY_i \sin\varphi_i & \cos\varphi_i \end{bmatrix} \quad (1)$$

The derivation of amplitude reflection (r) and transmission (t) coefficients is resulting in the following expressions:

$$r = \frac{Y_0 M_{11} + Y_0 Y_s M_{12} + M_{21} - Y_s M_{22}}{Y_0 M_{11} + Y_0 Y_s M_{12} + M_{21} + Y_s M_{22}} \quad (2)$$

$$t = \frac{2Y_0}{Y_0 M_{11} + Y_0 Y_s M_{12} + M_{21} + Y_s M_{22}} \quad (3)$$

where Y_0 and Y_s are the characteristic admittances of the media on both sides of the multilayer. M_{ij} are the elements of the characteristic matrix of the multilayer. Light is incident from the medium with admittance Y_0. The energy coefficients (reflectance, transmittance, and absorptance) are given as:

$$R = |r|^2 \quad (4)$$

$$T = \frac{Re(Y_s)}{Re(Y_0)} |t|^2 \quad (5)$$

$$A = (1 - R)\left[1 - \frac{Re(Y_s)}{Re[(M_{11} + Y_s M_{12})(M_{21} + Y_s M_{22})^*]}\right] \quad (6)$$

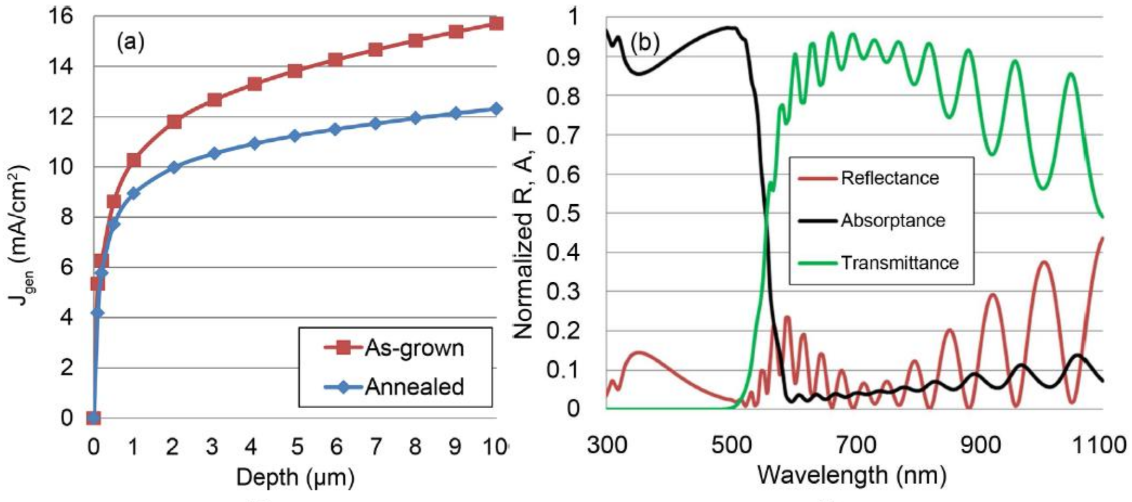
3. Simulation tools

This review article on tandem solar cells based on metal oxides and crystalline silicon considered the following simulation software tools: Silvaco, OPAL2 and MATLAB for optical modeling approach. These tools allowed to obtain useful results concerning optimization of the STHSC under investigation, as follows:

- OPAL2 simulation platform was used for evaluation of optical spectral characteristics, respectively reflectance, absorptance, and transmittance for different component layers of the STHSC.
- MATLAB software allowed the implementation of transfer matrix algorithm in order to analyze possible buffer layer materials for the STHSC from an optical point of view.
- Silvaco software contributed to the evaluation of dependence of photo-generated current on thickness of the absorber layer (Cu_2O) in order to establish the optimum thickness of such layer specific for the STHSC.

4. Results and Discussions

In the STHSC structure, the thermal losses are lowered if most high energy photons are absorbed in the top subcell, and therefore it is advantageous to absorb most of the high energy photons in the Cu_2O absorber layer. Figure 4(a) shows the modeled photogenerated current versus thickness for the as-grown and annealed Cu_2O layer under AM1.5G illumination. The calculation shows that an annealed Cu_2O layer of 2 μm thickness will yield about 10 mA/cm2 of photocurrent. This corresponds to approximately 80% of the photocurrent that can be generated for an infinitely thick Cu_2O layer. Figure 4(a) also shows that the photo generated current is lower for the annealed Cu_2O layer, when compared to the as-grown Cu_2O layer, because there is less grain-boundary scattering present. In general, annealing is required to enhance the electrical properties of the sputter-deposited Cu_2O absorber layer [12]. Figure 4(b) shows the calculated normalized reflectance, absorptance, and transmittance as a function of wavelength, using ray tracing method and the OPAL2 simulation platform [13]. In the modeled structure, an 80 nm thick front AZO layer, a 2 μm thick Cu_2O layer, and a 75 nm thick bottom AZO layer were implemented.

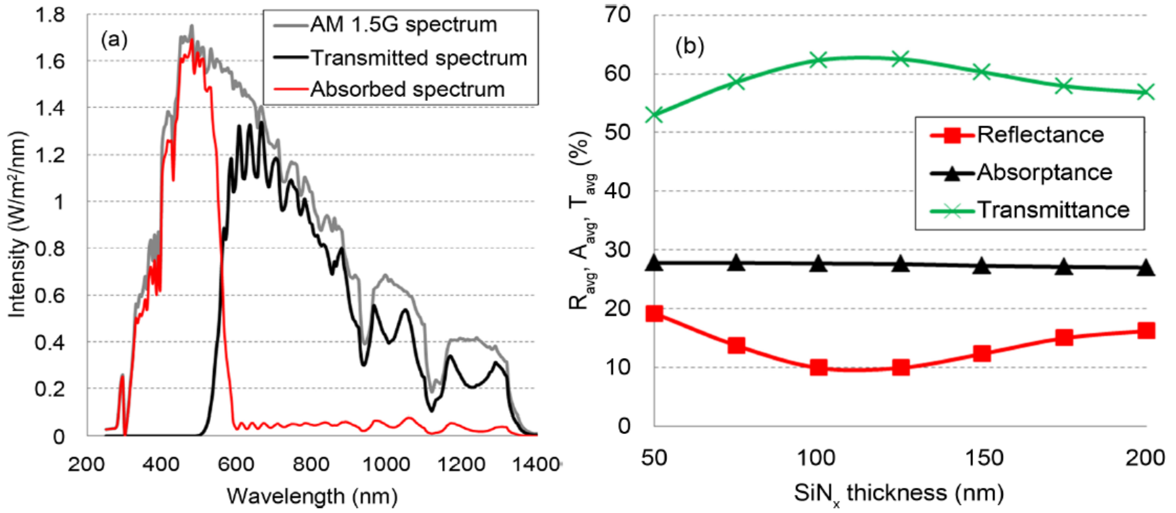


(a) (b)

Fig. 4. (a) Photogenerated current as function of depth for the Cu_2O absorber layer; (b) Normalized spectral reflectance (R), absorptance (A), and transmittance (T) for the ZnO/Cu_2O subcell [1].

The usual thickness of a SiN_x anti-reflection coating in a conventional c-Si solar cell is around 80 nm. Despite that, in a STHSC device the energy spectrum of photons going towards the c-Si bottom subcell is different compared to a conventional cell, since most short-wavelength photons are absorbed in the top subcell. Figure 5a shows the transmitted and absorbed spectral intensity for the ZnO/Cu_2O subcell. In order to allow the SiN_x layer to act as an effective antireflection coating, its thickness has to be increased to accommodate the photon spectrum shift towards longer wavelengths. The percentage of reflectance, absorptance, and transmittance in average, as a function of thickness for the SiN_x layer are depicted in Figure 5b. The simulation shows that the lowest reflectance and highest transmittance are obtained for around 120 nm thickness of the SiN_x layer. Increasing the thickness of the SiN_x layer from 80 nm to 120 nm, reduces total reflectance for the STHSC device from 12.7% to 9.7%.

A transfer matrix algorithm was implemented in MATLAB, for different buffer layer materials presented in Table 1, specifically ZnO, in order to analyze the absorptance and reflectance for the buffer layer (Figure 6a), respectively for the top ZnO/Cu_2O subcell (Figure 6b). The simulation presented in Figure 6a shows good absorptance in the upper range of the spectrum and low reflectance for the ZnO buffer layer. The algorithm was further applied to the metal oxide subcell, with the ZnO buffer layer implemented, in order to assess optical performance of the ZnO/Cu_2O heterojunction, as can be seen in Figure 6b. The optical performance is good, with over 80% absorptance in the visible spectrum range while the reflectance of the Cu_2O layer is low, in agreement with the literature [14, 15]. The peaks in the spectra can also be caused by material surface imperfections.



(a) (b)

Fig. 5. (a) Absorbed and transmitted spectral intensity for the ZnO/Cu_2O subcell; (b) Average reflectance (R_{avg}), absorptance (A_{avg}), and transmittance (T_{avg}) as a function of thickness for the SiN_x layer [1].

Table 1. Buffer materials implemented in the simulation [9].

Buffer material	Aff. (eV)	Eg (eV)	Eff (%)
ZnO	3.6	3.35	11.91
TiO_2	3.9	3.44	8.26
Ga_2O_3	4	5.18	8.92
CdS	4	2.40	8.45
$Zn(O_{0.25},S_{0.75})$	4.07	3.13	6.23
$Zn(O_{0.5},S_{0.5})$	4.45	2.83	2.8
$Zn(O_{0.75},S_{0.25})$	4.58	2.97	1.73
ZnS	4.5	3.50	3.97

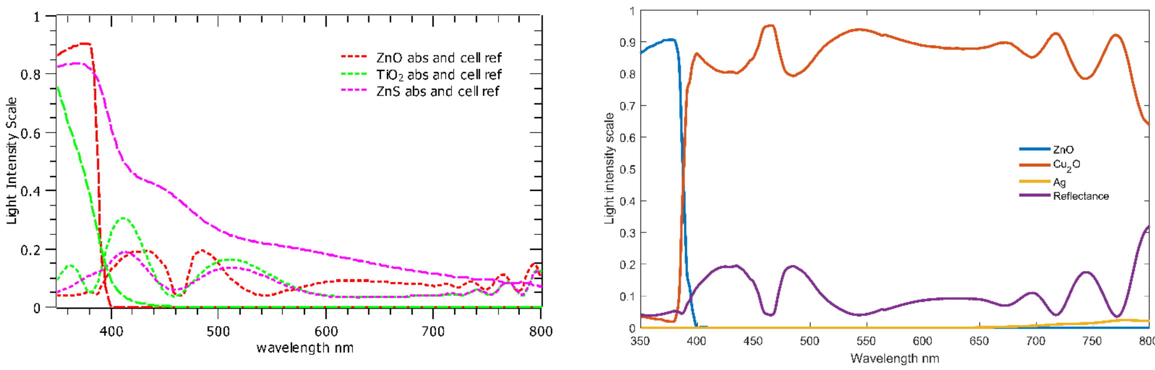


Figure 6. a) Buffer material absorptance and reflectance; b) Metal oxide top subcell absorptance and reflectance [10].

The modeling of the ZnO/Cu_2O subcell using Silvaco Atlas suggests that materials such as Zn(O,S), TiO_2, and Ga_2O_3 can be successfully implemented as buffer layer [16, 17], while providing a low conduction band offset for the heterojunction, shown in Table 1.

5. Conclusions

This review highlights the importance of using optical modeling and simulation tools for determining the optimum design for a silicon-based tandem heterojunction solar cell incorporating metal oxides [1, 4, 5, 9, 10, 14, 18].

Basic methods for optical modeling, namely ray tracing and transfer matrix algorithms, were applied.

Using several specialized simulation software, the optical spectral characteristics (reflectance, absorptance and transmittance) of the absorber, buffer and AZO layers, were determined and used to find the optimum layer thicknesses.

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