Application of a computationally efficient implementation of the RCWA method to numerical simulations of thin film amorphous solar cells

I. Semenikhin[1], M. Zanuccoli[2], M.Benzi[2], V. Vyurkov[1], E. Sangiorgi[2], C. Fiegna[2]

1 Institute of Physics and Technology RAS, 117218 Moscow, Russia
2 ARCES-DEIS University of Bologna & IUNET ,47521 Cesena (FC), Italy

Abstract-**This paper presents a new implementation of the Rigorous Coupled Wave Analysis (RCWA) method to model the propagation of electro-magnetic waves in nanostructured optoelectronic solid state devices like solar cells. The proposed method is based on an improved and computational efficient S-matrix approach that can be extended to three-dimensional geometries.**

I. INTRODUCTION

Modeling of optoelectronic devices and in particular solar cells requires an accurate prediction of the electromagnetic field map and of the optical generation rate per volume and time unit inside the absorbing media. Nano-metric structures like diffraction gratings or nanowires are adopted in advanced photo-voltaic devices in order to increase the light absorbance. In thin film (TF) solar cells with amorphous materials most interfaces between different media feature nano-sized roughness, therefore a rigorous numerical solution of the Maxwell equations is required to model the propagation of electromagnetic waves in such devices. Typical approaches to solve the Maxwell equations are the well-known time-consuming finite difference time division method (FDTD) and the rigorous coupled wave analysis (RCWA). The computational effort is one of the most serious open issues for FDTD and RCWA[1]. In this work we apply our implementation of the RCWA method to model accurately the light propagation in multi-layer devices featuring non-periodic geometries like randomly rough interfaces. In particular we calculate the electrical output parameters of a TF amorphous silicon (a-Si) solar cell by using the RCWA simulator to perform the optical simulation. The method will be extended in future to three dimensional problems; in this work we consider only two-dimensional (2-D) simulation domains.

II. SIMULATION DOMAIN AND OPTICAL PROBLEM

We consider electro-magnetic plane waves propagating in a 2D spatial domain and impinging on a multi-layer structure with both flat and rough interfaces, without any limitations in terms of amount of layers, geometrical features of the interfaces and thickness of the layers. The proposed method is based on the reformulation of the algorithm previously used to solve Schrödinger wave equation [2, 3].

RCWA is based on the expansion of the electromagnetic field and of the permittivity in terms of spatial harmonics and on a subsequent discretization along the vertical axis z (by assuming as step Δz) to solve a set of second order differential equations with respect to z [4] (Fig. 1A). The trade-off between accuracy and computational effort is based on a proper sizing of the number of Fourier modes and on Δz. In case of TE polarization (similar approach is adopted for TM) the equation to solve is:

$$\Delta E_y = -k_0^2 \varepsilon(x,z) E_y, \quad E_x = E_z = 0 \qquad (1)$$

$$k_0^2 = \varepsilon_0 \mu_0 \omega^2 = \omega^2 / c^2 = (2\pi/\lambda)^2$$

ε_0 and μ_0 are the electric permittivity and magnetic permeability of vacuum, λ and ω are the wavelength and the angular frequency, respectively. The approach described in [4], leads to the following solution of the problem:

$$E_y(x,z) = \begin{cases} \sum_{s=-\infty}^{\infty} \left(c_{1,s}^{+} e^{\mathrm{i}\sqrt{k_1^2-k_{xs}^2}(z-z_1)} + c_{1,s}^{-} e^{-\mathrm{i}\sqrt{k_1^2-k_{xs}^2}(z-z_1)}\right) e^{\mathrm{i}k_{xs}x}, & z \le z_1 \\ \sum_{s=-\infty}^{\infty} d_{1,s}\chi_{1,s}(x,z) + d_{2,s}\chi_{2,s}(x,z), & z_1 \le z \le z_2 \\ \sum_{s=-\infty}^{\infty} \left(c_{2,s}^{+} e^{\mathrm{i}\sqrt{k_2^2-k_{xs}^2}(z-z_2)} + c_{2,s}^{-} e^{-\mathrm{i}\sqrt{k_2^2-k_{xs}^2}(z-z_2)}\right) e^{\mathrm{i}k_{xs}x}, & z \ge z_2 \end{cases} \qquad (2)$$

$$k_{xs} = k_0(n_1 \sin(\theta) + s(\lambda/p)), \quad k_l = k_0 n_l, \quad l = 1,2$$

Functions $\chi_s(x,y,z)$ satisfy the equation (1) for TE polarization with the following boundary conditions:

$$\chi_{1,s}\big|_{z=z_1} = e^{\mathrm{i}k_{xs}x}, \quad \chi_{1,s}\big|_{z=z_2} = 0$$
$$\chi_{2,s}\big|_{z=z_1} = 0, \quad \chi_{2,s}\big|_{z=z_2} = e^{\mathrm{i}k_{xs}x} \qquad (3)$$
$$\chi_{i,s}(x+p,z) = e^{\mathrm{i}k_0 n_1 p \sin(\theta)} \chi_{i,s} \quad i = 1,2$$

After solving the equations (2)-(3) for $\chi_S(x,y,z)$ we find the coefficients $c_{l,s}$ and $d_{l,s}$ by matching the conditions:

$$E_y\big|_{z=z_i-0} = E_y\big|_{z=z_i+0}, \quad \frac{\partial E_y}{\partial z}\bigg|_{z=z_i-0} = \frac{\partial E_y}{\partial z}\bigg|_{z=z_i+0}, \quad i = 1,2 \qquad (4)$$

The multi-layer structure is split in homogenous (constant permittivity) and non-homogenous regions (non constant permittivity). To simplify the description of the algorithm we consider a spatial domain with only one non-homogeneous region, as sketched in Fig. 1A. Inside the non-homogenous region ($z_1 < z < z_2$), by using the S-matrix, we can write:

$$\begin{pmatrix} \mathbf{c}_2^{+} \\ \mathbf{c}_1^{-} \end{pmatrix} = \mathbf{S} \begin{pmatrix} \mathbf{c}_1^{+} \\ \mathbf{c}_2^{-} \end{pmatrix}.$$

The above mentioned algorithm is used to calculate **S**-matrix only within non-homogeneous regions. For homogeneous regions, the S-matrix is calculated analytically. The total S-matrix for the structure of M regions is given by $\mathbf{S} = \mathbf{S}^{(1)} \otimes \mathbf{S}^{(1)} \otimes \ldots \otimes \mathbf{S}^{(M)}$. This approach allows us to calculate very efficiently the electro-magnetic field inside multilayer structures featuring rough interfaces since we use numerical computations (2)-(4) only within the portions of the structure where roughness exists.

III. RCWA APPLICATION: TF SOLAR CELL SIMULATION

We investigated the dependence of the electrical output parameters of a TF a-Si solar cell on the roughness of the TCO/a-Si interface for the device of Fig. 1B, in which the a-Si is deposited on a SiO_2 substrate (1mm thick). The heights of the rough interface are described by a Gaussian distribution with correlation length equal to 25nm. Three values of roughness have been considered in this work: 0nm (flat interface), 25nm and 50nm. In the latter case the roughness is comparable to the total thickness of the absorbing layer (500nm). The simulated structure is 2μm wide.

For the optical simulation N=60 Fourier modes have been adopted and Δz has been set to 1nm. By using σ_{rms} as simulation parameters, the absorbed power in the a-Si layer has been calculated within the range 300nm-1000nm by assuming for each wavelength the electric field amplitude equal to E_0=500V/m. The results, reported in Fig. 2, show that the absorbed power increases for increasing roughness. The optical generation map per volume and time unit G_{opt} is calculated by assuming the input irradiance from the AM1.5G spectrum from 300nm up to 1000nm. Fig. 3 shows the G_{opt} maps inside the a-Si layer for σ_{rms}=25nm and σ_{rms}=50nm.

The electrical simulation is performed by a drift-diffusion simulator, by taking into account the recombination losses in the a-Si layer. The density of states as function of energy is described by exponential and Gaussian distributions of levels as discussed in [5] to take into account for realistic losses in the amorphous silicon.

TABLE I

OUTPUT PARAMETER CALCULATED BY THE ELECTRICAL SIMULATOR

σ_{rms} [nm]	Jph [mA/cm^2]	Jsc [mA/cm^2]	Voc [V]	FF	Eff [%]
0	15.34	12.19	0.897	56.42	6.17
25	17.40	13.62	0.902	56.88	6.98
50	17.84	12.82	0.897	58.00	6.67

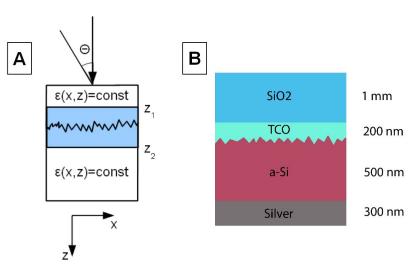

Fig. 1 (A) 2D sketch of the simulation domain with one non-homogeneous region; (B) Cross section of the simulated a-Si TF solar cell. The light is impinging on the SiO_2 layer. The roughness of the TCO/a-Si interface is denoted by σ_{rms}.

The photo-generated current density Jph (Tab. I) increases with the roughness consistently with the trend of the calculated absorbed power (Fig. 2). In addition, in Tab. I are reported the short circuit current density (Jsc), the open-circuit voltage (Voc), the Fill Factor (FF) and the efficiency calculated by the electrical simulator. It is worth notice that the maximum Jsc, the maximum Voc and consequently the maximum efficiency, are obtained for σ_{rms}=25nm while for σ_{rms}=50nm the Jsc, the Voc and the efficiency are lower than those for σ_{rms}=25nm; in fact, for larger roughness values, a larger optical generation occurs in the region close to the surface leading to larger values of Jph as well as larger recombination losses (the p-doped region is affected by defect densities larger than those of the intrinsic layer). Moreover, larger roughness leads to the larger area of the ITO/a-Si interface and therefore larger surface recombination occurs.

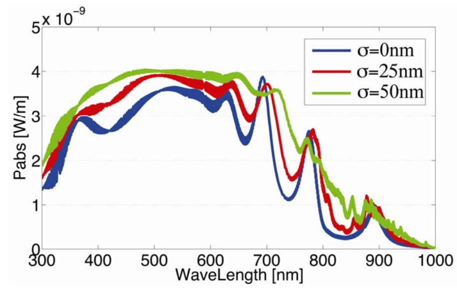

Fig. 2 Calculated absorbed power (P_{abs}) inside the a-Si layer for different values of roughness σ_{rms} of the TCO/a-Si interface. The amplitude of the incident electric field is 500 V/m.

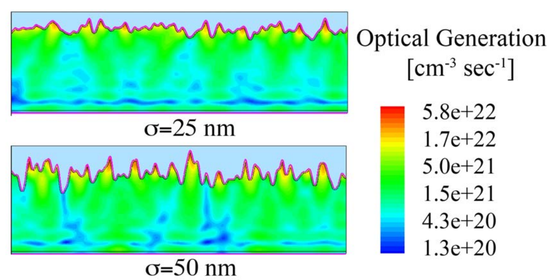

Fig. 3 Maps of the calculated optical generation rate inside the a-Si layer for different roughness σ_{rms} of the TCO/a-Si interface.

IV. CONCLUSIONS

We applied a computationally efficient implementation of the RCWA method to the analysis of multi-layer thin film solar cell featuring rough interfaces. Our implementation of the RCWA method, based on S-matrix, is a rigorous approach that can be used to model the propagation of the electromagnetic waves in nanostructured devices with arbitrary geometries and size. The method lends itself to straightforward extension to three dimensional problems leading to a speed-up of about 100 times with respect to other rigorous approaches like the FDTD. The results of the optical simulation have been coupled to a drift-diffusion simulator to investigate the dependence of the output parameters of the cell on the roughness of the ITO/a-Si interface.

ACKNOWLEDGMENT

Partially supported through the END project from the ENIAC Joint Undertaking under grant agreement n° 120214 and by the NANOFUNTION FP7-NOE.

REFERENCES

[1] J. J. Hench, Z. Strakos, Electr. Trans. Num. Analysis, Vol. 31, 2008.
[2] V. Vyurkov et al., Proc. SPIE, 7025, p. 70251K, (2008).
[3] A. Orlikovsky et al, in Nanoscaled Semiconductor-on-Insulator Structures and Devices, Springer, pp. 323-340, (2007).
[4] I. Semenikhin et al. , 14th IWCEI, pp. 187-190, 2010
[5] A, Fantoni et al., Mathematics and Computers in Simulations, Vol. 49, 1999