Advanced approaches in optical simulations of thin-film solar cells

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***Abstract*—In rigorous optical modeling and simulation of thin-film solar cells a few constraints and bottlenecks have been addressed recently. Two of them are related to how to include thick incoherent layers in the coherent finite element based simulations and how to describe and include non-conformal growth of layers in a thin-film solar cell. In this paper we present and apply three different solutions to speed up and improve the simulations of realistic thin-film solar cell in superstrate configuration: (i) solutions for including optically thick incoherent glass layer in superstrate type of solar cells and (ii) how to consider its thickness in millimeter range and and (iii) we present a non-conformal layer growth model. By applying these advanced features to 3-D optical modeling, it becomes possible to simulate the complete solar cell structures (incl. front glass) rigorously and time efficiently and to consider the realistic textures at all internal interfaces thus gaining in accuracy of simulations.**

I. Introduction

In simulation of optoelectronic devices (e.g. solar cells) the rigorous 3-D modeling based on finite element method (FEM) is gaining on attention lately. In the case of optical simulations of thin-film solar cells the simulations in frequency domain are to be more appropriate than simulations in time domain, since the measured material parameters and solar illumination spectrum can be easily imported into the optical models and the use of non-rectangular elements enables accurate description of nano-features of the cell (e.g. nano-textured interfaces). In simulations of thin film solar cells (TF-SC) in superstrate configuration (e.g. silicon based), the thick glass superstrate has often been excluded from the analysis. In this paper we highlight a solution how to include thick incoherent glass layer in rigorous FEM simulation by applying the *phase elimination* method and by scaling down its thickness to minimize the simulation domain [1]. In TF-silicon SC the rough interfaces are crucial to improve light scattering at interfaces and light trapping inside the active layer. Thus, solar cells are built on top of rough transparent conductive oxide (TCO) superstrates, such as SnO_2:F or ZnO, or substrates (e.g. nano-rough Ag contact). However, after the deposition of the layers of solar cell the base surface roughness is modified, therefore, the importance of non-conformal growth model [2] to be used in simulations will be highlighted. Such a model needs to reproduce the realistic change of roughness of internal interfaces the TF-silicon SC. We implement the presented approaches in the commercial software COMSOL Multiphysics® simulator [3], which is based on FEM, to simulate the complete TF-SC structures.

II. Numerical Model

In numerical model for optical simulation of TF-SC in COMSOL software we use perfectly matched layer (PML) boundary condition to close the top of the simulation domain in order to reduce the reflection of scattered light back into the model. The excitation was applied below the PML layer. At the bottom of Ag back contact layer, absorbing boundary condition was applied. On the sides of the simulation domain perfect magnetic or electric conductor was used to simulate the assumed symmetry of the structure, Fig 1.

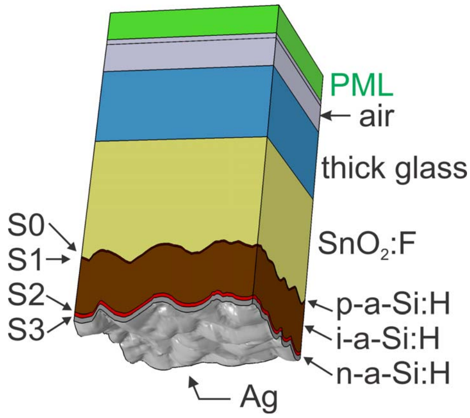

Fig. 1. Numerical model for an example of thin-film amorphous silicon (a-Si:H) single junction solar cell with thick incoherent glass layer (in figure its final, scalled down thickness is shown) and different surface/interface textures (S0 to S3) obtained by non-conformal growth model.

A. Non-conformal growth model

To model realistic interfaces between layers in the TF-SC a non-conformal growth model, which details are described in [2] was used for determination of surface textures inside the solar cell. The model is based on combination of conformal growth and vertical translation of the texture. In Fig. 2 the base surface (S0) of the SnO_2:F TCO (650 nm thick) is shown and was measured with the atomic force microscope (AFM) while the modified surfaces after deposition of p-a-Si:H (10 nm, S1), i-a-Si:H (300 nm, S2), n-a-Si:H (20 nm, S3) layers were obtained by applying the non-conformal growth model.

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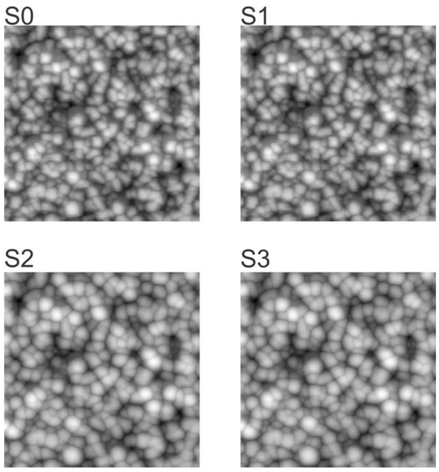

Fig. 2. Base surface (S0) as obtained from AFM measurement and the surfaces after the p- (S1) i- (S2) and n-layer (S3) of a-Si:H solar cell deposition, as obtained from the growth model.

B. *Incoherent glass layer*

The coherent models do not allow direct simulations of (thick) incoherent layers. Here we have used the *phase elimination method* [1] to handle a glass superstrate at the front side of the solar cell. This means that we made two simulation runs over the whole wavelength region: one run at fixed thickness of glass layer (*d*) and the other at shifted thickness (to eliminate the influence of the phase of light waves), which is also wavelength dependent (λ):

$$d'(\lambda) = d - Re[\frac{\lambda}{4N_{glass}(\lambda)}] \qquad (1)$$

where N_{glass} is complex refractive index of glass. The superposition is used to combine the results.

C. *Thinning of the incoherent glass layer*

Another problem of front glass superstrate is its thickness (usually 1 – 4 mm). The incoherent glass layer is very thick compared to TF-SC and modeling such thick glass layer in 3-D models would be impossible by today's hardware. Since the mesh for such layer would be far too large for today's computers, scaling the thickness of the incoherent glass layer is used [1] to minimize the simulation domain. By reducing the thickness of layer (d^*) the extinction coefficient of glass (k) needs to be modified according to the following equation to preserve the level of light absorption in the glass:

$$k^*(\lambda) = k^*(\lambda)\frac{d}{d^*} \qquad (2)$$

In our simulations we have reduced the thickness of glass from 1 mm to 500 nm (2000x). In this way the model size was greatly reduced while the modified extinction coefficient does not significantly affect the reflection of light at the front (air/glass) and back (glass SnO2:F) interface, since it is still much smaller than the real part of refractive index of glass.

III. Aplication of the Models

A complete a-Si:H thin-film solar cell in superstrate configuration was simulated using the COMSOL simulator considering all the features described above. The simulations were done in the wavelength region where the a-Si:H solar cell is active – between 400 – 800 nm with the step size of 10 nm. The measured complex refractive indices of materials were used in simulations. Considering ideal extraction of generated charge carriers from i-layer and neglection the contribution from p- and n-doped layers the simulated absorptance of i-layer can be directly compared to external quantum efficiency, EQE, of the cell [4]. Good agreement is obtained between measured and simulated EQE of a-Si:H solar cell for the whole wavelength region, Fig 3. In results of simulations no interference fringes from the thick glass layer are observed (as in measurements), which means the method for inclusion of incoherent layers in coherent models has successfully filtered them out. Using the calibrated non-conformal layer growth model in simulations the scattering level of light, affecting the intensity of interference fringes, is matched more accurately as well.

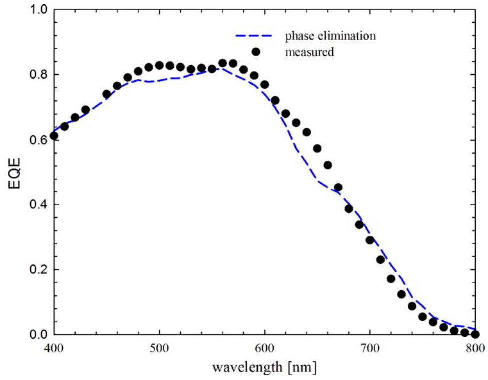

Fig. 3. Measured EQE of a-Si:H solar cell (symbols) compared to simulated absorptance in i- layer of a-Si:H solar cell (dashed line).

IV. Conclusion

We have demonstrated two selected advanced approaches in rigorous optical modeling of thin-film solar cells. The complete a-Si:H solar cell with thick glass superstrate and the realistic surface roughness of different interfaces was simulated in FEM based simulator utilizing our advanced approaches. Good agreement is obtained between 3-D simulations and measurements of EQE.

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VI. References

[1] A. Campa, J. Krc, and M. Topic, "Two approaches for incoherent propagation of light in rigorous numerical simulations," Progress In Electromagnetics Research, Vol. 137, pp. 187-202, 2013.

[2] M.Sever et al., "Combined model of non-conformal layer growth for accurate optical simulation of thin-film silicon solar cells", submitted for publication. Solar Energy Materials and Solar Cells.

[3] Available: http://www.comsol.com

[4] J. Krc, M. Zeman, O. Kluth, F. Smole, and M. Topic, "Effect of surface roughness of ZnO:Al films on light scattering in hydrogenated amorphous silicon solar cells", Thin Solid Films, Vol. 426, No. 1-2, pp. 296-304, 2003.