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Optical Model with Combined Ray and Wave Optics for Optimization of Textures of Thin-Film Solar Cells

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Abstract: We extended the capabilities of our GenPro4 solar cell optical model, making it an even more powerful tool for nanotexture optimization. We show its application to thin-film CIGS, silicon, and perovskite/silicon tandem solar cells. © 2022 The Author(s)

1. Introduction

Dedicated optical models are essential tools for the modelling of the next generation of solar cells. These models predict the spectrally resolved absorptance in each layer of a solar cell and identify parasitic absorption and reflection losses. The main challenge is the accurate modelling of light scattering by surface textures. Textures of various shapes and sizes are implemented in solar cells to improve both in-coupling and trapping of light. Our GenPro4 optical model [1] treats textures with feature sizes much smaller than the wavelength of sunlight (<<1 μm) using the built-in scalar scattering model [2], and textures with feature sizes >>1 μm using the built-in ray-tracing model. In this work, we introduce an additional scattering model for periodic, intermediate-sized (~1 μm) textures, based on three-dimensional (3D) rigorous coupled wave analysis (RCWA) [3]. For each interface, each of these different scatter models can be selected. We show how the extended GenPro4 model can be used to optimize textures compatible with thin-film solar cell technologies, such as copper indium gallium di-selenide (CIGS), thin-film silicon (TF-Si) and perovskite.

2. Optical Model Validation

GenPro4 built-in models calculate the bidirectional scatter distribution function (BSDF) of each textured interface, both for p- and s-polarized light [1]. An RCWA model, capable of calculating this BSDF from a given texture height profile, was integrated into GenPro4. To validate this 3D RCWA model, we calculated the BSDF of a one-dimensional binary grating and compare it to the diffraction angles predicted by the grating equation. Fig. 1a, shows that there is excellent agreement on the calculated diffraction angles (θ_{out}) for a given incident angle (θ_{in}). A second validation is performed by simulating textured ultra-thin CIGS solar cell shown in Fig. 1b. In a previous study we calculated the CIGS absorptance of this device using a finite element (FEM) based Maxwell solver [4] (blue line Fig. 1c). The absorptance obtained from our 3D RCWA model agrees very well (red dots in Fig. 1c), demonstrating its accuracy. Note that all results shown here are for unpolarized sunlight.

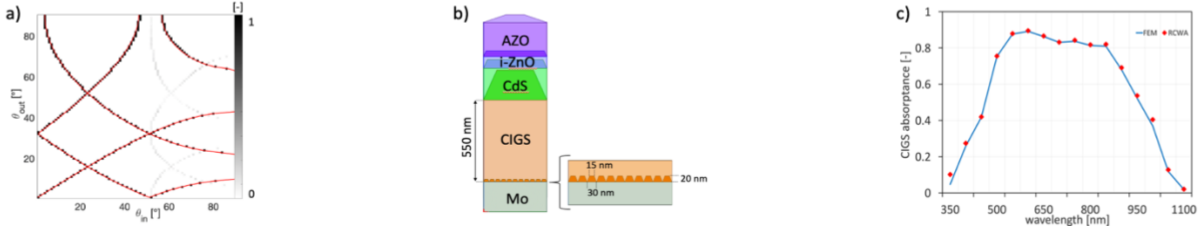

Figure 1: a) BSDF of a binary grating calculated using RCWA model (black) and grating equation (red); b) cross-section of front and rear textured CIGS solar cell; c) corresponding absorptance in CIGS layer calculated by RCWA and FEM Maxwell solver (reference) models.

3. Results

3.1 Thin-film silicon triple junction solar cells

We modelled a TF-Si triple junction solar cell, consisting of three p-i-n junctions, with amorphous and micro-crystalline silicon as active layers (see Fig.2a). The interfaces have a micro-texture (see Fig.2b) selected to enhance the light trapping while providing a suitable deposition substrate [5]. GenPro4 was used to simulate the absorptance of the total device (see Fig. 2c, orange line) as well as the absorptance in the top, middle and bottom absorber layers (blue, green, red lines) and their sum (black line). A comparison between the built-in ray-tracing-model (solid lines) and the scalar scattering model (dashed lines) shows significantly higher absorption predicted by the ray-tracing model. This shows the known limitations of the scalar scattering model to model the enhanced in-coupling effect, which is more pronounced for this type of texture with larger features.

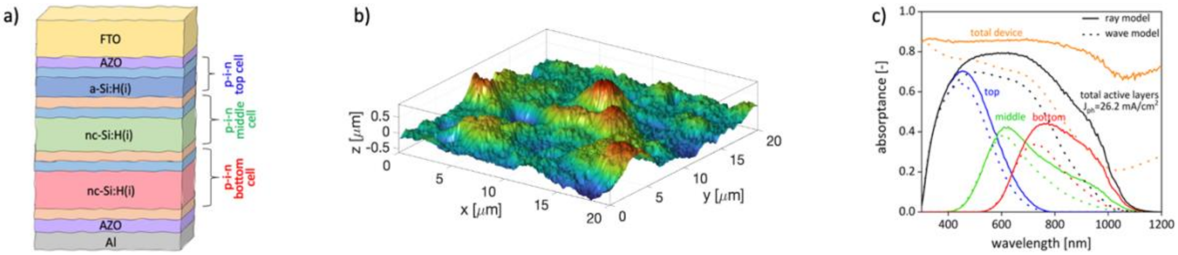

Figure 2: a) Cross-section of thin-film silicon triple junction solar cell; b) measured surface texture used as input for the simulations; c) simulated absorptance of top, middle and bottom absorber layers (blue, green, red), their sum (black) and total device absorption (orange) calculated using ray/wave model (solid/dashed).

3.2 Perovskite / silicon tandem solar cells

We also modelled monolithic perovskite / silicon tandem solar cells, consisting of a thin-film perovskite top cell, deposited on a nano-textured silicon wafer based bottom cell (see Fig. 3a). Note that introducing some type of nano-texture seems essential for achieving record tandem efficiency [6] but the optimum morphology of such a texture is still a topic of investigation [7,8]. We use the fast GenPro4 algorithm to systematically scan through various front texture sizes and shapes, analyzed using the RCWA model, while treating the fixed rear pyramid texture with the ray-tracing model. For example, for a sine-wave texture with 300 nm period, increasing texture amplitude from 0 (planar) to 200 nm enhances the blue response of the perovskite top cell, which increases its implied photocurrent by 0.6 mA/cm^2 (see Fig. 3b). During fabrication, perovskite deposition is non-conformal, meaning that the texture amplitude at perovskite front (A_1) and rear sides (A_2) typically differ. We scan through all combinations of A_1 and A_2, showing that the highest total implied photocurrent of over 40 mA/cm^2 is obtained when both A_1 and A_2 are maximized (see Fig. 3c). Note that amplitudes larger than 200 nm might result in even larger optical gains but could deteriorate the electrical performance and were therefore not included in this study.

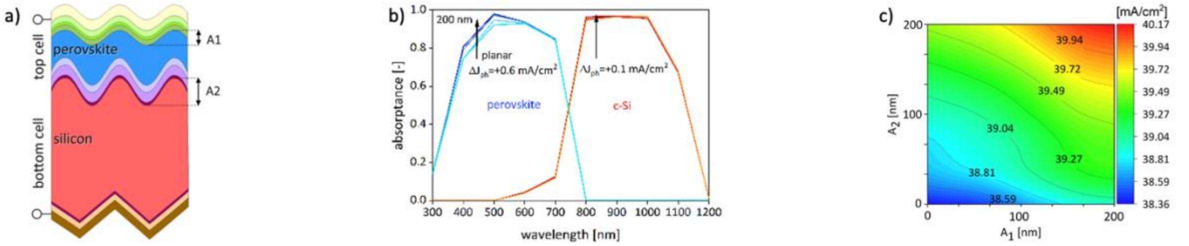

Figure 3: a) Cross-section of perovskite silicon tandem, with nanotexture amplitudes A_1 and A_2 at perovskite front and rear side; b) simulated absorptance in perovskite (blue) and silicon (red) for increasing texture amplitude for the conformal case $A_1 = A_2$; c) Total implied photocurrent (perovskite + silicon) for every amplitude combination.

4. Conclusions

We extended the capabilities of our GenPro4 model by integrating an RCWA model, making it a powerful tool for optimization of thin-film textures. Here we have only briefly shown the application of the extended model to thin-film CIGS, silicon, and perovskite / silicon tandem solar cells. At the conference we will show more detailed optimization studies, revealing new insights that can accelerate the optimization of the next generation solar cells.

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