Accurate optical simulations of periodic nanostructures on a thick glass substrate

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***Abstract*—The air-glass interface of periodically nano-textured thin-film solar cells can strongly affect the total reflectivity. However, in many rigorous Maxwell solvers, it is not considered directly. Here, we discuss two *a posteriori* corrections that account for the air-glass interface and we compare the numerical results to experimental data.**

Keywords—diffraction gratings, antireflection coatings, optical simulations, solar energy.

I. Introduction

Optical simulations allow to improve the understanding of photovoltaic and other optoelectronic devices. Hence, they can help to optimize device designs. To perform this task, reliable and accurate simulation tools are vital. Rigorous Maxwell solvers, such as the finite element method (FEM), are well suited to treat nanostructured periodic thin-film stacks. The characteristic length of unit cells, which can be treated with FEM at optical wavelengths, is limited to few micrometres. However, nanostructured thin-film stacks often are deposited onto a glass superstrate (thickness ~ 1 mm), which cannot be treated accurately with FEM.

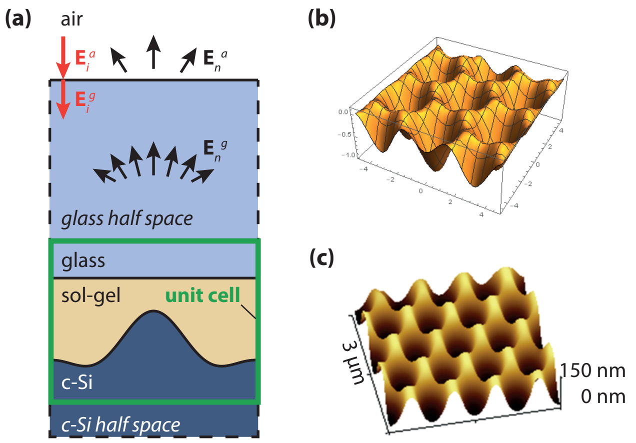

Fig. 1: (a) Cross section through a periodic unit cell with a sinusoidal interface [1] and the glass and silicon half spaces above and below the unit cell. The *first-order correction* accounts for the interaction of the glass-air interface with light, which is reflected from the unit cell into the glass half space. The sketch depicts all the electric field components needed for this calculation. (b) The negative cosine texture used in the simulations [1]. (c) Atomic force microscopy (AFM) measurements of a sinusoidally nanotextured sol-gel layer on glass with 750 nm pitch and about 150 nm texture height, hence an aspect ratio of about a = 20%.

Dr. Klaus Jäger received his PhD cum laude (with distinction) from Delft University of Technology (TU Delft) in November 2012. After one year at the Dutch company HyET Solar he spent another year as postdoc at TU Delft, where he worked on an educational book on Solar Energy. In January 2015 he became a postdoc in Christiane Becker's Young Investigator Group Nano-SIPPE at Helmholtz-Zentrum Berlin. Klaus is mainly interested in numerical and theoretical work on nanophotonics for solar energy applications.

Under normal incidence, an air-glass interface reflects about 4% of the incident light. When the investigated system does not scatter strongly, it is sufficient to take solely these 4% into account (0th order correction). But if the nanotexture reflects a significant fraction of the light back into the glass superstrate at large angles, reflection of this light by the glass-air interface back into the nanostructure may become important (1st order correction).

In this contribution, we will discuss the two corrections and test them for silicon on glass with a hexagonal sinusoidal nanotexture, as illustrated in Fig. 1. The findings presented in this manuscript are presented in greater detail in [2].

II. The two corrections

Periodically structured thin-film layer stacks reflect and transmit light into discrete and well-defined diffraction orders. The reflectivity R of the structure, shown in Fig. 1(a), into the glass halfspace can be calculated with

$$R(\lambda) = \frac{1}{\left|\mathbf{E}_i^g(\lambda)\right|^2 \cos\theta_i^g(\lambda)} \sum_n \left|\mathbf{E}_n^g(\lambda)\right|^2 \cos\theta_n^g(\lambda), \quad (1)$$

where the electromagnetic field components E^g and the angles θ^g are output from the Maxwell solver. The subscript i denotes the incident wave and the superscript g denotes fields and angles in glass, as depicted in Fig. 1(a). The sum is taken over all channels into which the structure reflects.

The zeroth-order correction accounts only for the initial reflection of the air-glass interface. The reflectivity in air R^0 is calculated using

$$R^0(\lambda) = R(\lambda)[1 - R^g(\lambda)] + R^g(\lambda), \quad (2)$$

where the superscript 0 denotes the zeroth-order correction, R^g is the reflectivity of the air-glass interface and λ is the wavelength.

The first-order correction takes into account that not all the light, which is reflected from the layer stack into the glass half space, is transmitted into air but that a part is reflected back into the layer stack by the glass-air interface. For its calculation, the electric field vectors $\mathbf{E}_n^a$ and angles θ_n^a in air must be derived using the Fresnel equations and Snell's law, respectively,

$$R^1 = \frac{1}{\left|\mathbf{E}_i^a\right|^2 \cos\theta_i^a} \sum_n \left|t_n^s \mathbf{E}_{s,n}^g + t_n^p \mathbf{E}_{p,n}^g\right|^2 \cos\theta_n^a + R^g. \quad (3)$$

Here, we must decompose the $\mathbf{E}_n^g$ vectors into s- and p-polarized components and multiply them with the Fresnel coefficients t_n^s and t_n^p, respectively. These transmission coefficients describe waves that are transmitted from glass into air. In contrast, $\mathbf{E}_n^a$ is connected to $\mathbf{E}_n^g$, which is used in Eq. (1), via transmission from air into glass.

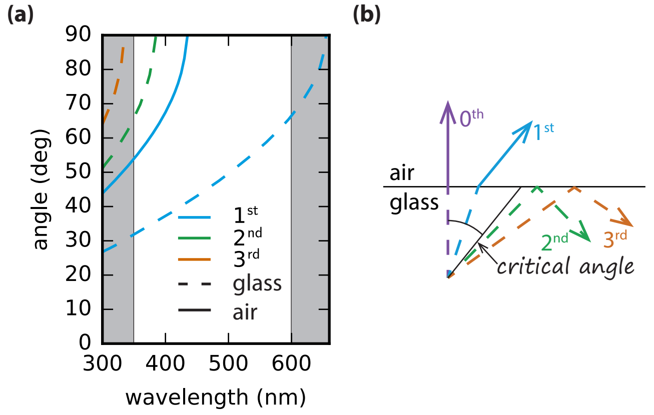

Fig. 2: (a) Angles of the diffraction orders into which a hexagonal periodic structure with a pitch of P = 500 nm scatters light at normal incidence. The figure shows the angles in glass and in air. The zeroth diffraction order ($\theta_g = \theta_a \equiv 0$) is not shown. The experimentally-relevant wavelength range (350 – 600 nm) is depicted. In glass, the diffraction orders are present up to much longer wavelength than in air, which is also in (b).

III. Numerical and experimental details

We performed FEM simulations on the sinusoidally textured layer stack, depicted in Fig. 1(a), with the package JCMsuite [3], as described in Ref. [1]. Experimentally, the sinusoidal nanotextures were prepared on glass with nanoimprint lithography [4]. Subsequently, an about 10 µm thick nanocrystalline silicon layer was deposited, which then was liquid-phase crystallized with a laser [5].

IV. Results

Figure 2 shows the angles of the different diffraction orders in glass and air for light that is refracted by hexagonal periodic structures with 500 nm pitch at normal incidence. The zeroth-order $(\theta_g = \theta_a \equiv 0)$ is not shown. In glass, the different diffraction orders are present until much longer wavelength than in air, as illustrated also in Fig. 2(b).

Figure 3(a) shows numerical and experimental 1 – R spectra for a nanotextured sample with 500 nm pitch. Large differences are seen between the two corrections. The numerical results are shown for the angles of incidence of Simulation results are shown for two angles of incidence: $\theta_{\text{in}} = 0°$ and $\theta_{\text{in}} = 8°$. Measurement data are for $\theta_{\text{in}} = 8°$. We observe that the $\theta_{\text{in}} = 8°$ curve matches much better with the measured data than the curve for normal incidence.

Figure 3(b) shows the mean 1 – R for the two corrections and experimental data as a function of the aspect ratio a of the nanotexture and two different pitches at $\theta_{\text{in}} = 8°$. The mean is taken between 350 and 600 nm wavelength. The first-order correction resembles the experimental data much better.

V. Conclusions and outlook

The 1st-order correction allows to obtain reflectivity spectra, which match very well with experimental data.

Despite the excellent agreement between measurements and simulations, also the effect of higher order corrections must be studied. Further, currently the first order correction approach only allows to correct reflectance spectra but it cannot be applied for correcting the absorptance in layer stacks with multiple absorbing layers yet.

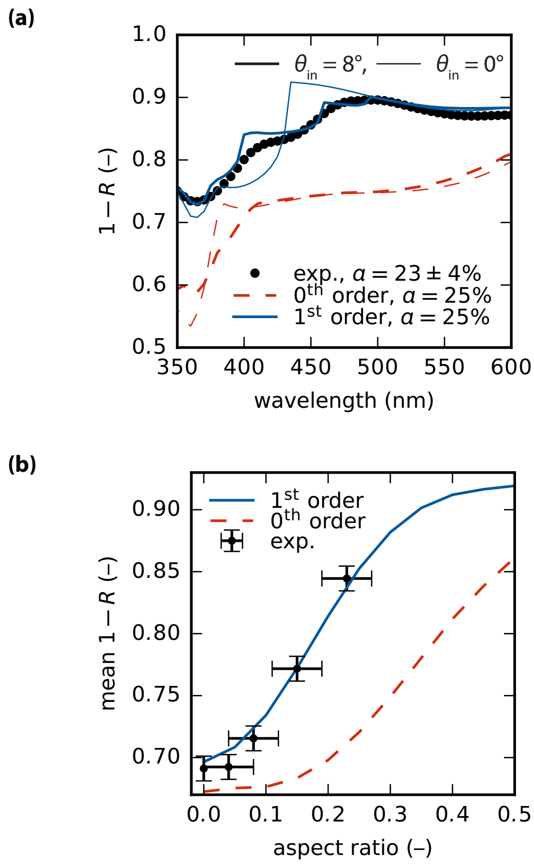

Fig. 3: (a) Numerical and experimental 1 – R spectra for the nanotextured layer stacks illustrated in Fig. 1. Numerical results were calculated with the 0th- and 1st-order corrections, as defined in Eqs. (2) and (3), respectively. The two corrections differ because not all diffraction orders that are present in glass can propagate into air [see Fig. 2]. Simulation results are shown for two angles of incidence: $\theta_{\text{in}} = 0°$ (thin lines) and $\theta_{\text{in}} = 8°$ (thick lines). Experimental results were obtained with $\theta_{\text{in}} = 8°$. (b) Mean 1 – R between 350 and 600 nm wavelength obtained with the two corrections and for experimental data at $\theta_{\text{in}} = 8°$. The first-order correction results match much better with the experimental data. All results were obtained with 500 nm pitch.

References

[1] K. Jäger, C. Barth, M. Hammerschmidt, S. Herrmann, S. Burger, F. Schmidt, and C., *Optics Express* **24**, A569 (2016).

[2] K. Jaeger, M. Hammerschmidt, G. Köppel, S. Burger, and C. Becker, "On Accurate Simulations of Thin-Film Solar Cells With a Thick Glass Superstrate," in Light, Energy and the Environment, Leipzig, Germany (Optical Society of America, November 2016), paper PM3B.5.

[3] J. Pomplun, S. Burger, L. Zschiedrich, and F. Schmidt, *Phys. Status Solidi B* **244**, 3419 (2007); http://jcmwave.com.

[4] G. Köppel, B. Rech, and C. Becker, Nanoscale **8**, 8722 (2016).

[5] J. Haschke, D. Amkreutz, and B. Rech, Jpn. J. Appl. Phys. **55**, 04EA04 (2016)