Sinusoidal Nanotextures for Enhanced Light Management in Thin-Film Solar Cells

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***Abstract*—We present a numerical study on sinusoidal gratings for efficient coupling of light into a silicon absorber. In contrast to square gratings, hexagonal gratings exist with great variety; we show that their morphology strongly affects in-coupling of light – even if their period and height is kept constant. Sinusoidal nanotextures are a promising tool to enhance coupling of light into optical devices with large refractive index contrasts.**

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

I. Introduction

Every highly efficient solar cell requires *light management*, which consists of two aspects that have to be taken into account: (1) efficient *coupling* of light into the absorber and (2) *trapping* of light that is not absorbed during its first pass through the absorber. While light trapping is especially important for weakly absorbing materials, such as crystalline silicon (c-Si), which is an indirect bandgap material, efficient coupling of the incident light into the absorber is important for *all* solar cell concepts.

In this document, we summarize the numerical development of *square* and *hexagonal* sinusoidal gratings for maximized coupling of the incident light into a solar cell absorber.

The results are presented for liquid phase crystallized (LPC) c-Si thin-film solar cells that are developed at Helmholtz-Zentrum Berlin [1–4] and currently have an efficiency record of 12.1% [5]. However, sinusoidal nanotextures also can be beneficial for the coupling efficiency of other solar cell types, e.g. perovskite solar cells or CIGS solar cells. Because of different complex refractive indices, the optimal geometry will be different for the different technologies.

The results presented in this summary are published in much greater detail in [6].

II. Method

A. Mathematical description of sinusoidal gratings

Square and hexagonal gratings can be mathematically described with the equations

$$f_{\mathrm{sq}}(x, y) = \cos x \cos y, \tag{1}$$

$$f_{\mathrm{hex}}(x, y) = \cos[\tfrac{1}{2}(x + \sqrt{3}y)] \cos[\tfrac{1}{2}(x - \sqrt{3}y)] \cos(x + \varphi), \tag{2}$$

respectively, and are illustrated in Fig. 1. The *structure phase* φ allows us to generate a large variety of hexagonal gratings. Here we discuss gratings with $\varphi = 0$ ("cos"), $\varphi = \pi/2$ ("sin") and $\varphi = \pi/2$ ("−cos"). Note that for square gratings a similar phase shift only causes a lateral shift of the texture, but leaves the morphology unchanged. The period P and the height h of the gratings are set by vertical and lateral stretching.

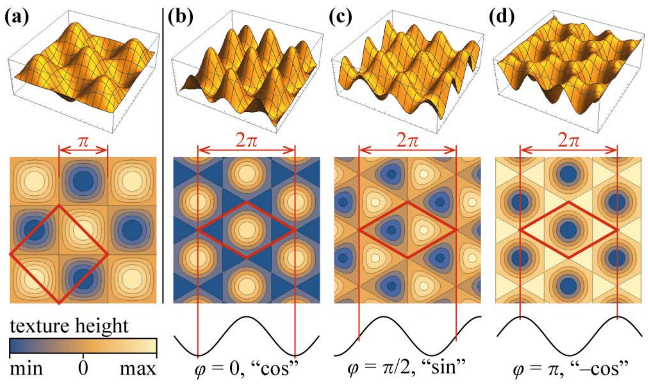

Fig. 1: (a) A square sinusoidal grating, as in Eq. (1). (b)–(d) Three different hexagonal sinusoidal gratings, as in Eq. (2). The functions depicted at the bottom of (b)–(d) illustrate the third term of the function in Eq. (2).

B. Details of the numerical simulations

We numerically studied, how the period P, the aspect ratio a ($a = h/P$) and the different morphologies affect coupling of the incident light into the silicon absorber, using the 3D unit cell shown in Fig. 2: an infinite half space of glass is covered by a sol-gel layer, which carries the nanotexture. The nanotexture is covered by a half space of crystalline silicon.

Using a Si half space is necessary, because we want to study only the coupling of light into the silicon. A silicon slab with finite thickness would become transparent at long wavelength and hence a part of the light would be reflected from its back surface and thus make an interpretation of the in-coupling process more difficult.

We solved Maxwell's equations with appropriate source, material and boundary condition settings, using a time-harmonic finite-element (FE) solver (JCMsuite) [7]. The infinite half spaces were simulated using *perfectly matched layers* on top and

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bottom of our structure. This allowed us to keep the glass thickness and the silicon thickness above the structure low at 100 nm and 200 nm, respectively and hence considerably reducing the computational cost of the simulations. The sides of the unit cells were treated with periodic boundary conditions.

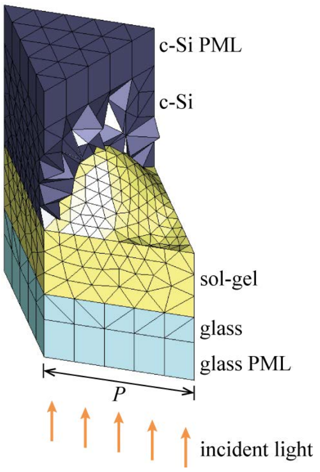

Fig. 2: The layer stack used for this study. Using *perfectly matched layers* (PML) on top and bottom allows us to treat the glass and c-Si layers as infinite half spaces while keeping the computational demand of the simualtions low.

As a figure of merit we used the *maximum achievable photocurrent density* J_{ph}^{max}, which is obtained by multiplying the fraction of light coupled into the silicon absorber with the photon flux obtained from the AM 1.5G spectrum [8], integrating over the relevant wavelength spectrum between λ = 300 nm and 1107 nm (the bandgap wavelength of c-Si) and multiplying with the elementary charge.

III. Results

Figure 3(a) shows J_{ph}^{max} of light coupled into the silicon absorber for the four different morphologies and a constant aspect ratio of a = ½. While the period clearly affects J_{ph}^{max}, the effect of the morphology on J_{ph}^{max} is even larger. Especially the "−cos" grating outperforms the other three morphologies for all investigated periods. For all four morphologies, the maximum lies around 500 nm – 600 nm. Except at P = 350 nm, the square grating performs worst for all periods. We can understand this when we realize that light can couple to *four channels* per diffraction order for square gratings but to *six channels* per diffraction order for hexagonal gratings.

We have not yet fully understood, why the "−cos" grating outperforms all the others. However, we observe that the "−cos" grating acts as an array of microlenses, as obvious from Fig. 3(b), which shows the imaginary part of the electric field energy density $\Im(w_e) = \Im(\frac{1}{4}\mathbf{E}\cdot\mathbf{D}^*)$ for P = 500 nm, h = 250 nm and at a wavelength of λ = 500 nm. Note that $\Im(w_e)$ is proportional to the absorbed power density [9]. We can clearly see that $\Im(w_e)$ is very strong in the focal region of the grating. For the "cos" and "sin" gratings, the maximally observed $\Im(w_e)$ is lower, as discussed in [6]. There we also show that the fraction of the in-coupled light is highest for "−cos" across the whole wavelength range.

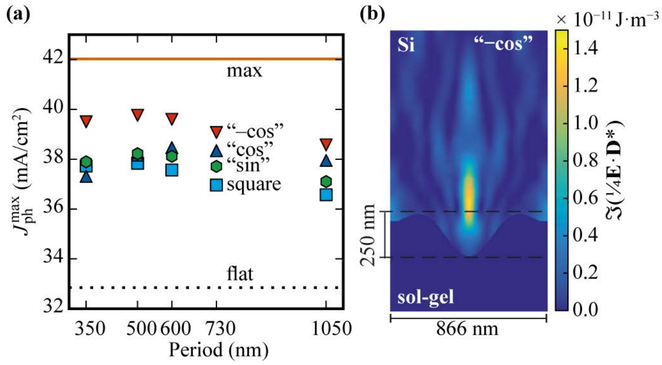

Fig. 3: (a) The maximum achievable photocurrent density J_{ph}^{max} of light coupled into the silicon absorber for the four different morphologies shown in Fig. 1 and an aspect ratio of $a = h/P$ = ½. As references also results for a flat sample (h = 0) and maximal in-coupling (all the light is coupled into Si) are shown. The reflectance of the front air-glass interface of about 4% was subtracted *a posteriori*. (b) The imaginary part of the electric field energy density $\Im(w_e) = \Im(\frac{1}{4}\mathbf{E}\cdot\mathbf{D}^*)$, which is proportional to the absorbed power density, for the "−cos" structure. Results shown for P = 500 nm, h = 250 nm and at a λ = 500 nm.

IV. Conclusions

We have numerically demonstrated that sinusoidal gratings are well-suited to strongly enhance coupling of light into a silicon absorber. Mathematically, various types of hexagonal textures can be generated (Fig. 1). Simulation results reveal that the so-called "−cos" performs best for all investigated periods (Fig. 3). With this grating the maximal achievable photocurrent density J_{ph}^{max} is increased by 7.0 mA/cm^2 for a period of P = 500 nm and a structure height of h = 250 nm. While the maximally achievable gain is smaller for layer stacks with additional antireflective layers (3.6 mA/cm^2), the overall J_{ph}^{max} is larger [6].

The next steps will be to extend these simulations to full LPC-Si solar cell stacks with a limited absorber thickness of 10 µm in order to take also effects from the solar cell back side into account. Further, the results observed numerically also should be evaluated experimentally.

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