Broadband Absorption in Thin Films Motivated by Strong Light Bending

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Photon management toward the absorption over a wide spectral range of the solar light is important to various absorption-based photonic devices. The key for high absorption in thin films is the ability to “bend the light” from the normal direction into the in-plane direction. Broadband absorption enhancement is reported in thin films decorated with top surface light funnel arrays (LF arrays) due to strong bending of the light by the arrays into the films, in contrast with excitation of thin films by top surface nanopillar arrays (NP arrays) that is governed by forward scattering. The broadband absorption in the film below the LF array (LF film) is 40% higher than that in a film below an optimized NP array (NP film). Also, the strong light bending by the LF arrays into the underlying film induces strong absorbivity peaks substantially exceeding the Yablonovitch limit for both the LF film and the total array–film complex. Finally, the superior LF film broadband absorption is due to strong light bending from the normal direction into the in-plane direction which is manifested in efficient generation of mode hybridizations.

1. Introduction

Optical absorption of the sun radiation over a wide spectral range is paramount to various technologies spanning from absorption-based photonic devices[1–3] to sun power conversion.[4–6] For example, extremely thin solar cells with absorption similar to bulk material exhibit low recombination currents and higher photovoltaic efficiencies.[7,8] and support the utilization of rare materials for photovoltaic technology. Yablonovitch suggested random decoration of the front and back interfaces of a thin dielectric slab to maximize the slab capacity for trapping light, and used statistical ray optics to define the $4n^2$ limit for light trapping, where $n$ is the slab dielectric constant.[15] More recently, wave optics was used to describe light trapping in thin films, and has been the loci of both theoretical and experimental research work. Sturmburg et al. demonstrated an approach for improved absorption in free-floating silicon nanopillar (NP) arrays, and showed light trapping that is governed by pairing of photonic states to the impinging illumination, medium power concentration in the NPs, and substantial Fabry–Perot resonances.[16] Lin and Povinelli reported absorption governed by high field concentration inside the NPs coupled with excitation of guided resonance modes in sparse free-floating NP arrays,[17] and Shalev et al. numerically showed that absorption in free-floating NP arrays is optimized using relatively wide NPs with low absorption cross section.[18]

It was numerically shown in various works that surface subwavelength gratings can potentially provide momentum components to the incident illumination by diffraction, for example, thereby exciting guided modes in the underlying absorbing substrate.[19–21] Sheng et al. theoretically demonstrated light trapping beyond the $4n^2$ limit in thin films decorated with a top subwavelength grating, as the presence of the grating entails an increase in the photonic states density.[22] Yu et al. theoretically described light trapping in a thin slab decorated with a 2D shallow subwavelength grating on top, and argued that the $4n^2$ limit can be exceeded once the number of slab waveguide states is maximized and the number of diffraction orders is minimized.[23,24] Callahan et al. argued that to surmount the $4n^2$ limit, the population of the photonic states need to be higher than the population of local states in the respective bulk material.[25]

Light trapping exceeding the $4n^2$ limit and absorption improvement over a wide spectral range of the solar light was shown for arrays composed of subwavelength gratings of a semiconductor material.[16,18,26–41] Wallentin et al. showed a 13.8% photovoltaic efficiency for arrays composed of InP NPs by surpassing the $4n^2$ limit,[43] and Fountaine et al. showed an ultrahigh absorption in NP arrays of InP.[40] Spinelli et al. reported a near-unity absorption with arrays of subwavelength Mie resonators due to forward scattering by the arrays into the underlying films,[40] Huang et al. demonstrated reflectivity lower than 1% for silicon nanotip arrays,[46] and Jeong et al. fabricated a thin photovoltaic cell using nanocone grating with extremely low levels of reflection.[47]
We recently introduced absorption of the solar light based on light funnel (LF) arrays, where a LF is a subwavelength structure in the shape of a cone that is “bottom-side-up” relative to the impinging light.[45,46] Broadband absorption and efficient light trapping was also reported for other inverted structures such as compound parabolic concentrators[47,48] and inverted hyperboloids.[49] The optical coupling between the top surface LF arrays and the underlying films was also reported, and the contributions of film absorption and array absorption to the overall complex absorption were examined.[50–52] In this study, we investigate the strong film excitation generated by the presence of top surface LF arrays, and particularly the efficient light bending by the LF arrays from the vertical direction into the in-plane direction which concludes significant absorption enhancement of the underlying film.

2. Results and Discussion

Figure 1a shows the transition from a NP array–film complex (NP complex) into a LF array–film complex (LF complex) which is accomplished by the decrease in the NPs bottom diameter. In this work, we consider a film thickness of 100 nm, an array height of 200 nm, a LF bottom diameter (D_L) of 200 nm and the LF top diameter (D_s) and the NP diameter are fixed at 400 nm, as shown in Figure 1a. Figure 1b shows the numerically calculated absorptivity spectra of a LF complex and a NP complex, where the period (P) of the arrays is fixed at 500 nm. Also, the absorptivity spectra of a 300 nm-thick silicon thin film and the corresponding Yablonovitch limit are presented. Figure 1c shows the decoupled LF and NP arrays absorptivity spectra, the absorptivity of a 200 nm film and the corresponding Yablonovitch limit. Similarly, Figure 1d shows the decoupled absorptivity of the film below the LF array (LF film), the decoupled absorptivity of the film below the NP array (NP film), the absorptivity of a 100 nm film and the corresponding Yablonovitch limit. As expected, the complexes as well as the decoupled films and arrays present absorptivity that is considerably superior to the absorptivity of a corresponding undecorated thin film. This superiority is particularly accentuated for the decoupled films. Note that, as expected, the absorptivity at the short wavelength range is dominated by the NP and the LF arrays. More interestingly, while the absorptivity of the complexes and the arrays are similar, the absorptivity of the LF film is significantly more pronounced than the absorptivity of the NP film. Specifically, note the two high LF film absorptivity peaks at wavelengths 640 and 760 nm (760 nm peak significantly exceeds the Yablonovitch limit) that govern the respective absorptivity peaks of the LF complex, marked in dashed circles in Figure 1b,d. The broadband absorption efficiency (\(\eta\)) is the absorptivity spectra weighted with the AM 1.5G solar spectrum (Experimental Section). The insets of Figure 1b–d show the broadband absorption of the complexes (\(\eta_{\text{comp}}\)), the broadband absorption of the decoupled arrays (\(\eta_{\text{array}}\)), and the broadband absorption of the decoupled films (\(\eta_{\text{film}}\)). Note the overall increase in >12% for the LF complex compared with the NP complex which is due to the 40% increase in the LF film as compared with the NP film. Figure 1e shows the absorbed photon density (\(\eta_{\text{abs}}\)) and the magnitude of the time-averaged Poynting vector (|S|) of the LF complex at \(\lambda = 640\) and 760 nm, respectively. The apparent homogeneous optical excitations of the LF film at \(\lambda = 640\) and 760 nm suggest strong light bending by LF array into the LF film. To address this light bending mechanism, the optimal array period for broadband absorption is identified next.

Figure 2a shows the broadband dependency on array periodicity for the NP and LF complexes, and for the corresponding decoupled arrays and films. Interestingly, the NP complex \(\eta_{\text{comp}}\) and the LF complex \(\eta_{\text{comp}}\) are similar for the range of selected periodicities and an overall decrease in \(\eta_{\text{comp}}\) is apparent with increasing P for both systems, as was reported previously.[18,46] However, the highest \(\eta_{\text{comp}}\) is recorded for a LF complex of P = 550 nm with a 13% increase compared with the respective NP complex \(\eta_{\text{comp}}\). Also, note that for the full range of selected periodicities, the NP array \(\eta_{\text{array}}\) is higher than the LF array \(\eta_{\text{array}}\). Whereas the LF film \(\eta_{\text{film}}\) is higher than the NP film \(\eta_{\text{film}}\) for most of the selected periodicities. Specifically, for P = 550 nm the LF film \(\eta_{\text{film}}\) is 40% higher than the NP film \(\eta_{\text{film}}\), and it is 33% higher than the highest NP film \(\eta_{\text{film}}\) at P = 540 nm. Figure 2b shows \(\eta_{\text{abs}}\) under AM 1.5G solar irradiation for the LF complex and the NP complex for periods of 1000 and 550 nm: LF film excitation away from the LFs is evident, whereas the NP film is mostly excited directly below the NPs, and whereas for P = 1000 nm, the \(\eta_{\text{abs}}\) of the NP and the LF films looks similar, consistent with Figure 2a, for P = 550 nm, the higher LF film \(\eta_{\text{abs}}\) is evident. Figure 2c shows the current density depth profile under broadband solar illumination as a function of distance from the top of the arrays for various P values (see Experimental Section). Evidently, the film current densities for P = 500 and 550 nm are significantly higher for the LF film compared with the NP film throughout the full volume of the film. This enhancement decreases appreciably with increase in P. Finally, Figure 2d shows the optical length enhancement in the LF films as function of P (see Experimental Section); consistent with Figure 2c, the optical length enhancement is most accentuated for small P values.

Figure 3a shows the LF complex absorptivity spectrum decoupled into the LF array absorptivity spectrum and the LF film absorptivity spectrum for P = 550 nm. Figure 3b shows the respective spectra for the NP complex for P = 550 nm. Next, we examine the origin of the five highest absorptivity peaks of the LF film and the five highest absorptivity peaks of the NP film marked in Figure 3a,b, respectively. Two straightforward observations are noted: 1) It is apparent that the LF film peaks are higher than the NP film peaks, and 2) as shown in Figure 3a,b insets, the ratio between the film absorptivity (\(A_{\text{film}}\)) and the array absorptivity (\(A_{\text{array}}\)) of the selected five peaks is significantly higher for the LF complex. These two observations suggest of a more efficient film excitation by the LF array. Figure 3c shows the |S| and the \(S_x\) and \(S_z\)-components of the time-averaged Poynting vector (\(S_x\) and \(S_z\), respectively) for the five NP complex absorptivity peaks. \(S_x\) reflects the amount of “light bending” from the normal direction into the lateral direction (\(S_z\) behavior is similar). Note, that for all five absorptivity peaks \(|S|\), \(S_x\) and \(S_z\) indicate that NPs excite the film immediately below them. This forward scattering by the NP arrays into the underlying substrate was also described by others.[38] Figure 3d shows the corresponding distributions of the five highest absorptivity peaks of the LF film. Clearly, the LF array induces \(S_x\) in the film that provides a more homogeneous |S| distribution, and hence a higher
extent of “light bending” with the resulting higher interaction length and a higher film absorptivity. Therefore, while forward scattering is the main excitation mechanism in the NP film, the more homogeneous excitation of the LF film suggests excitation of traveling waveguide modes. The effect of “light bending” is clearly validated in Figure 3e, which shows the ratio between the film lateral components $(S_x + S_y)_{film}$ and the array lateral components $(S_x + S_y)_{array}$ for the five peaks for both the NP and the LF complexes. For the NP complex, the ratios are slightly higher than unity with highest value of 1.75. On the other hand,
the LF complex ratios are significantly higher with highest ratio reaching 5.3. This reflects the increase in the LF film lateral components which is synonymous with the notion of “light bending” in the film induced by the presence of the LF array.

To identify the absorption mechanism, Figure 4a,b shows the absorptivity as a function of photon energy and the reciprocal lattice constant, \( \beta = 2\pi/P \), for the LF film and NP film, respectively. The respective array periods and wavelengths are indicated as well. Well-defined narrow lines of strong dispersion are displayed for both complexes where the higher LF film absorptivity along these lines is indicative of a greater extent of light bending in the LF film. The higher absorptivity of the LF film for periods smaller than \( \approx 700 \) nm, and the decrease in absorptivity with increasing \( P \) is consistent with previous reports.[18] The strong dispersion lines could reflect the excitation of slab waveguide modes that yields an elevated interaction length and absorptivity.

To this end, the dispersion relation of an asymmetric slab waveguide is calculated with a bottom air layer and a top mixed silicon/air dielectric layer that is calculated using mean-field theory.[54,55] As shown in Figure 4a,b, only the fundamental mode \( \text{TM}_0 \), presented in a dotted white line, overlaps to some extent with one of the strong numerical dispersion lines for both the LF and the NP films; hence, several of the dispersion points along this line reflect the excitation of pure slab-guided modes. As for LF2 and NP2, although seemingly overlap the \( \text{TM}_0 \) line, still the distributions shown in Figure 3c,d suggest mode hybridizations rather than excitation of the \( \text{TM}_0 \) mode. The disagreement between the remaining numerical dispersion lines and the analytical slab waveguide solutions suggests that these numerical dispersion lines also reflect mode hybridizations. The strong absorption peaks NP1, NP3-5 and LF1, LF3-5 and clearly overlap the respective numerical dispersion lines, which are consistent with the distributions shown in Figure 3c,d, suggests also that these peaks are dominated by mode hybridizations.

3. Conclusion

LF arrays provide a promising approach for a powerful absorption scheme of the solar radiation. Presently, we showed excellent broadband absorption in a thin silicon film induced by the optical pairing of the LF array and the film. We show that mode hybridizations govern the absorption of both the LF film and the NP film. However, the LF film is more tuned to light bending, whereas the NP film excitation is dominated by forward scattering. The absorption performance of LF arrays can be further amplified with the integration of broadband and omnidirectional antireflection schemes involving the decoration with other subwavelength structures.[56–58] Low-cost fabrication is of the utmost importance to any energy-harvesting application and particularly to photovoltaic technologies. Low-cost fabrication of subwavelength arrays was demonstrated using colloidal lithography[59,60] and particularly for LF arrays.[45] Currently, the fabrication of large LF arrays (square centimeters) is being developed based on nanoimprint lithography and dry etch, and therefore, albeit the complex etching required for LF array, the fabrication of such arrays can be realized using low-cost fabrication techniques. In this study, we examine silicon LF arrays, but the paradigm of LF arrays can be potentially applied to any photoactive material of choice. Furthermore, the utilization of top surface LF arrays allows efficient carrier extraction[61,62] as well as the realization of various strategies for carrier collection such as all-back...
Figure 3. a) The decoupled LF array absorptivity and decoupled LF film absorptivity for $P =$ 550 nm. The strong absorption peaks are marked as LF1–LF5. Inset: The inset presents the $A_{array}/A_{film}$ ratio for the strong marked absorptivity peaks. b) Same as (a) only for the NP complex. c) $|S|$, $S_y$, and $S_x$ for the selected five absorptivity peaks of the NP complex. The direction of the electric field of the impinging illumination is indicated. d) Same as (c) only for the LF complex. e) The ratio between the film lateral components ($S_x + S_y$)$_{film}$ and the array lateral components ($S_x + S_y$)$_{array}$ for both the NP and the LF complexes.
contacts, axial junction configuration, and radial junction configuration. We believe that LF arrays are an additional important milestone toward efficient photon management for solar harvesting and photonic applications.

4. Experimental Section

The methods are detailed in the Supporting information. In short, The Sentaurus electromagnetic wave solver by Synopsys Inc. was used for the 3D finite-difference time-domain computations. A single unit cell in a square-tiled array was calculated with a periodic boundary condition (BC) along the x-y directions, where the BC is for a normally x-axis-polarized plane wave. Complementary perfectly matched layers BC is provided along the z-axis which excludes reflections from the bottom of the complexes. The numbers of reflected, transmitted photon, and absorbed photon are calculated at each wavelength using detectors positioned below and above the cell, and the reflectivity, transmissivity and absorptivity are extracted, respectively. The calculations are executed for wavelengths 400–1100 nm. For reliable calculations, the mesh size is smaller than 0.1 of the wavelengths in the material. The spatially distributed time-averaged Poynting vector ($S$) and the absorbed photon density are spectrally calculated. The broadband absorption efficiency ($\eta$) is the weighted average of the absorptivity and the solar spectrum (AM 1.5G). The broadband current density assumes that every absorbed photon generates an electron–hole pair ($e^–h^+$) that is successfully delivered to the external load by the contacts. The spatial distribution of the current density is calculated for 10 nm slices for both the arrays and the films. The broadband optical length enhancement is calculated by normalizing the integrated absorbed photons in the LF film by the integrated absorbed photons in the NP film.

The material constants of silicon are taken from the study by Palik.[53] The analytical solutions of the asymmetric slab waveguide modes are taken from the study by Kogelnik,[54] and the effective medium theory considered for the effective index of refraction of the top mixed layer of air and silicon LF arrays is taken from the study by Astrova et al.[55]

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Research data are not shared.

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