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Plasmonic versus dielectric enhancement in thin-film solar cells

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Several studies have indicated that broadband absorption of thin-film solar cells can be enhanced by use of surface-plasmon induced resonances of metallic parts like strips or particles. The metallic parts may create localized modes or scatter incoming light to increase absorption in thin-film semiconducting material. For a particular case, we show that coupling to the same type of localized slab-waveguide modes can be obtained by a surface modulation consisting of purely dielectric strips. The purely dielectric device turns out to have a significantly higher broadband enhancement factor compared to its metallic counterpart. We show that the enhanced normalized short-circuit current for a cell with silicon strips can be increased 4 times compared to the best performance for strips of silver, gold, or aluminium. For this particular case, the simple dielectric grating may outperform its plasmonic counterpart due to the larger Ohmic losses associated with the latter.

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The discovery of extraordinary optical transmission through subwavelength apertures in metal films1 has lead to intense studies of plasmonic structures during the last decade.2 The extreme light concentration of plasmonic structures has been used in a range of applications such as sensors,3 optical lenses, ultrafast and compact photodetectors and modulators, near-field scanning optical microscopy, and in nonlinear optics.4

Plasmon excitation and light localization have been used to enhance the optical absorption in a number of different thin-film photodetectors and solar cell structures.5,6 Reference 7 suggests a systematic approach to increase the absorption in a thin Si film over the solar spectrum by distributing Ag strips on top of a SiO2-coated Si film on a SiO2 substrate. The Ag strips scatter the incident wave and allow the coupling to slab-waveguide modes in the Si thin-film. It is shown that the normalized short-circuit current for the solar spectrum is significantly larger and increased by up to 168% when strips of Si are used instead of the three different metals. It appears that the same optical mode localizations in the absorbing Si film are obtained for Si strips compared to metal strips, but without the undesired additional energy loss associated with the latter. This shows that the predominant enhancement for this particular case does not come from plasmon-mediated field enhancement, but rather from coupling made possible by the structured surface itself. Clearly, when benchmarking the performance of plasmon-enhanced absorption in planar Si thin films, attention should be paid also to the alternative of metallic structuring, such as surface-structuring of the Si itself.

The geometry of the periodic solar cell is shown in Fig. 1. A numerical model of the cell is based on full-wave finite element frequency domain (FEFD) simulations using COMSOL.12 The direction of the incoming optical wave,
governed by the time-harmonic Helmholtz equation,\textsuperscript{13} is perpendicular to the surface. The Si layer $\Omega_{Si}$ with thickness $a = 50 \text{ nm}$ absorbs a part of the optical energy calculated by the expression ($\Omega_{Si}$ excludes the Si strips in case of dielectric gratings)

$$\Phi = \frac{1}{2} \omega \varepsilon_0 \varepsilon_r \int_{\Omega_{Si}} |E|^2 \, \mathrm{d}r,$$

where $\omega$ is the angular frequency, $\varepsilon_0$ is the vacuum permittivity, $\varepsilon_r$ is the relative permittivity of the material, and $E$ is the electric field. The top and bottom part of the cell is terminated by perfectly matched layers (PML), see Ref. \textsuperscript{14} and the insert in Fig. 1, and the left and right boundaries are periodic with a period $p$ that can vary. The strip at the surface of the solar cell with thickness $t = 60 \text{ nm}$ and width $w = 80 \text{ nm}$ can consist of the 5 individual materials Ag, Au, Al, Si, and SiO$_2$. When the strips consist of Si, the thin layer of SiO$_2$ with thickness $s = 10 \text{ nm}$ is removed between the strip and the Si layer. The thickness of the SiO$_2$ substrate is 200 nm.

The absorption enhancement plots in $\Omega_{Si}$ for each of the 5 strip materials compared to a cell with a bare surface is calculated as function of the reciprocal lattice constant and the photon energy. The wavelength dependent dielectric constant $\varepsilon_r$ for Si is taken from Ref. \textsuperscript{15}; for SiO$_2$, it is found in Ref. \textsuperscript{16}, and the values for the metals are from Ref. \textsuperscript{17}. The absorption enhancements for the cell with an Ag strip for $E_z$ and $H_z$-polarized light are plotted in Figs. 2(a) and 2(c), respectively. The color scale is logarithmic, and areas between green and red indicate situations where the absorption is larger than for a bare surface. The plots correspond well to the plots in Ref. \textsuperscript{7}, and the small differences are due to different numerical methods used and possibly slightly different choices of material values and geometry parameters. When the absorption plots are made for Au and Al strips, the plots are similar to the ones for Ag. This indicates that the three metals result in the same effects and are coupling to the same slab-waveguide modes. The corresponding absorption enhancements are plotted for Si strips in Figs. 2(e) and 2(g). Compared to Ag strips, a greater part of the absorption enhancements are plotted for Si strips in Figs. 2(e) and 2(g)), but the enhanced modes in the case of Si strips spread over wider intervals. Finally, if the enhancement plots are made for SiO$_2$, they show an almost uniform distribution of a light green color corresponding to a performance slightly better than for a bare surface and only dim indications of first and second order mode patterns for the two polarizations can be seen. The modes are not well localized because the refractive index contrast between SiO$_2$ and air is relatively small.

The absorption enhancements from Figs. 2(a), 2(c), 2(e), and 2(g) indicate that somewhat similar slab-waveguide modes are generated for both metal and Si strips, i.e., the waveguide is only perturbed weakly by the addition of the dielectric or metallic nanostructuring. In order to compare them, four representative modes are plotted in

FIG. 2. Left column: Maps of the absorption enhancements in a Si thin film ($a = 50 \text{ nm}$) as a function of reciprocal lattice constant $G = 2\pi/p$ and photon energy $h\omega$. (a) and (c): Results for Ag strips and $E_z/H_z$. For example: Results for Si strips. The highest short-circuit current is indicated by a vertical line ($p = 279 \text{ nm}$ for Ag and $p = 249 \text{ nm}$ for Si). For field patterns associated with points a–d, see panels (a)–(d) in Fig. 3. Right column: Plots of corresponding relative losses in the strips for the Ag and Si cases, respectively.
Figs. 3(a)–3(d)—corresponding to the four points marked in Figs. 2(a)–2(d). The values for the cell period \( p \) and the optical wavelength \( \lambda \) are indicated in each case. Pairwise, the modes in metal and Si gratings are very similar. When the modes for Si strips are compared to the ones above for Ag, it is clear that the slab-waveguide modes of the same order and with similar field patterns can be generated no matter if the strips are formed by Si or metal. Hence, the enhanced absorption for this particular case is driven by grating effects, rather than plasmonic field enhancement. The optical field does not overlap much with the metal, but even small overlaps cause significant Ohmic loss. The overlap between the optical field and the Si strip is in general larger than for the metal, but still less energy is dissipated in this case.

In order to compare the broadband performance of the solar cell for the five different strip materials, the normalized short-circuit current is plotted as function of the cell period in Fig. 4(a). The shape of the curve for Ag is similar to the one from Ref. 7 and its maximum value 141% is found in Fig. 4(a). The shape of the curve for Ag is similar to the one from Ref. 7 and its maximum value 141% is found in Fig. 4(a). We use the standard AM1.5 (air mass) spectrum for the solar input. The performance for Al is similar to Ag, whereas Au does not provide any enhancement of the normalized short-circuit current compared to the bare cell, which is mainly due to higher values of the imaginary part of \( \varepsilon_r \) for the shorter wavelengths. However, Si performs better than the three metals for all cell periods, and it is better than the bare cell for almost the entire period interval considered. The curve reaches the highest value 268% for \( p = 249 \) nm, and the enhancement is, therefore, 4 times larger than for the best performance of the metals. When using SiO\(_2\) strips, the normalized short-circuit current is slightly better than the bare surface for the entire interval, but Si, Ag, and Al still reach higher maximum values.

To ensure that the better performance of Si is not governed by strongly localized resonances, a study of the dependence of strip thickness \( t \) is performed for Ag and Si. In Fig. 4(b), the best point from the normalized short-circuit current graphs is plotted for a number of values of \( t \). The two points marked with a circle in Fig. 4(a), therefore, correspond to the points marked with a circle in Fig. 4(b) for \( t = 60 \) nm. The individual value of the cell period is indicated for each point. This study again confirms that Si performs better than the metals. Other geometric parameters (like, e.g., the thickness of the SiO\(_2\) film between metal and Si) could likewise be optimized, however, our goal here is not to find the absolute optimum, but rather to illustrate the importance and potential gain from considering purely dielectric alternatives to plasmonic gratings.

In summary, a theoretical study of a periodic thin-film solar cell has been presented, where strips of Ag, Au, Al, Si, and SiO\(_2\) on top of the cell have been employed to enhance the absorption in a Si layer. It is shown that similar enhancements can be obtained for strips of metals and Si because similar localized mode effects are generated in the structure. However, less energy is lost in the Si strips and, therefore, the enhancements are in general greater and less dependent on cell dimensions and wavelength. This leads to larger values of the normalized short-circuit current for the Si strips. SiO\(_2\) strips only show slightly better performance compared to a bare surface because the refractive index contrast is too low to support localized modes. The study shows that for this particular device, a purely dielectric grating outperforms the plasmonic-based counterpart, primarily due to decreased Ohmic losses. Hence for the particular geometry, we do not observe any of the advantages usually associated with metallic gratings. Other test cases have led to similar conclusions although we cannot rule out the possible existence of cases...
where plasmon enhanced surfaces perform better than purely dielectric ones. In general however, we conclude that when evaluating the potential of absorption enhancements for plasmonic structures, attention should be paid to dielectric surface structuring as well in order to make technologically sensible comparisons and ensure the best possible technological solutions.

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