Enhanced absorption of thin-film photovoltaic cells using an optical cavity

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Enhanced absorption of thin-film photovoltaic cells using an optical cavity

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We show via numerical simulations that the absorption and solar energy conversion efficiency of a thin-film photovoltaic (PV) cell can be significantly enhanced by embedding it into an optical cavity. A reflective hemi-ellipsoid with an aperture for sunlight placed over a tilted PV cell reflects unabsorbed photons back to the cell, allowing for multiple opportunities for absorption. Ray tracing simulations predict that with the proposed cavity a textured thin-film silicon cell can exceed the Yablonovitch (Lambertian) limit for absorption across a broad wavelength range, while the performance of the cavity-embedded planar PV cell approaches that of the cell with the surface texturing.

1. Introduction

Photovoltaics (PV) offer a promising answer to the challenge of a renewable energy future[1]. Even with significant progress in recent years, efforts are being made to reduce cost even further so that PV can reach parity with conventional fossil fuels without government subsidies[2]. One approach to cost reduction is using thin-film crystalline silicon (c-Si) PV cells, which use significantly less high-quality silicon material than traditional cells[3]. The silicon wafer typically accounts for 30% - 40% of the total module cost, and this cost can be reduced if less material is used[4,5].

The drawback of thin-film cells is that incident photons have a shorter travel distance through the material than in traditional cells, yielding a lower chance of being absorbed. Tiedje and Yablonovitch, et. al. established an absorptance limit for silicon PV cells as a function of cell thickness (the “Yablonovitch limit” or “Lambertian limit”)[6]. This absorptance limit can be combined with the Shockley-Queisser limit (for example) to predict a solar to electricity conversion efficiency limit[7]. Absorptance in the Yablonovitch limit assumes incident photons are perfectly coupled (100% transmittance) into the cell and scattered isotropically at the front and back surfaces of the cell. Photons which would otherwise escape from the cell are trapped inside the cell if they have been scattered into an angle exceeding the critical angle (total internal reflection). This results in longer photon path lengths through the cell and therefore higher chance of absorption[8]. The absorption limit \( A \) is given by:

\[
A(L) = \frac{\alpha(L) L}{\alpha(L) L + \frac{1}{F}}
\]

where \( \alpha(\lambda) \) is the wavelength dependent absorption coefficient of the PV material, \( L \) is the cell thickness, and \( F \) is the absorption enhancement factor. The absorption enhancement factor is \( 4\pi^2 \) in the Yablonovitch limit, where \( n \) is the PV refractive index. Substituting this into Eq. (1) yields the familiar form of the Yablonovitch limit:

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Figure 1 Diagram of the PV cell cavity enhancement concept. Sunlight incident on a tilted cell that is not absorbed is reflected back to the cell, yielding more opportunities for absorption. Important geometric parameters include: aperture acceptance angle $\psi$, cell tilt angle $\gamma$, cell radius $r_{cell}$, and cavity radius $r_{cav}$.

The geometry of the cavity is an oblate ellipsoid, with the relationship between the semi-major axis $r_{cav}$ ("radius" of the ellipsoid) and semi-minor axis $h$ ("height" of the ellipsoid) given by

$$r_{cav} = \sqrt{h^2 + r_{cell}^2}$$

where $r_{cell}$ is the radius of the PV cell in the cavity. This geometry is used because it ensures that any ray originating from the PV cell that is specularly reflected from the ellipsoidal cavity will return to the PV cell[24,25]. The ellipsoid is tilted along with the cell such that its minor axis remains orthogonal to the PV cell, in order to preserve the previously mentioned geometrical reflecting property. Slight variations to this configuration (e.g., ellipsoid minor axis aligned with incident sunlight, a hemispherical cavity, etc.) were investigated and found to have marginally lower performance, so the results for those studies will not be reported here.

Cavity performance is predicted using ray tracing, which is a Monte Carlo technique that can be used to evaluate the radiative properties of systems[26]. Rays representing incident solar radiation are incident on the PV cell, with location and incidence angle determined by randomly generated numbers and the appropriate weighting functions. Based on the cell absorptance, the rays have a chance of being absorbed or reflected specularly (our optical simulations detailed below show that higher order surface diffractions are negligible for the investigated structured surfaces, see Appendix A). The rays are propagated through the cavity until all rays have been absorbed by the cell ("absorbed"), absorbed by the cavity walls ("mirror losses"), lost through the aperture ("aperture losses") or absorbed by the cavity floor ("floor losses"). The effective absorptance $A$ of the cell embedded into the cavity is given simply by

$$A = \frac{N_{cell}}{N_{inc}} \cos \gamma$$

where $N_{cell}$ is the number of rays absorbed at the cell, $N_{inc}$ is the total number of rays incident on the cell, and $\gamma$ is the tilt angle. The $\cos \gamma$ term accounts for effective area losses due to the incident sunlight not being normal to the cell.

There are three primary geometric parameters of the cavity to optimize for achieving high absorption and energy conversion efficiency: the acceptance angle of the cavity aperture, the tilt angle of the PV cell, and the size ratio of the cavity radius to the PV cell radius (all shown in Fig. 1). Another important cavity parameter is the wall specular reflectance, which is assumed to be 95%, a value which is achievable in the relevant spectral range using conventional metal coatings[27].

The cavity aperture acceptance angle, defined as the angle between a line from the edge of the PV cell to the near edge of the aperture and a normally incident ray from the sun, determines the maximum solar concentration ratio achievable at the cell[28]. It should be noted that this cavity aperture acceptance angle (shown in Fig. 1 as $\psi$) is different from the acceptance angle typically used in CPV applications, which refers to the tolerance of concentrating optics to misalignment. Larger cavity acceptance angles allow for higher concentration ratios but reduce the cavity effectiveness by allowing more photons to escape through the aperture. A fixed acceptance angle of 5° is used in this study, which allows for moderate concentration ratios (up to 360 suns).

Tilt angle is an important parameter to consider because if the cell is not tilted then most photons reflected from the cell leave the cavity through the aperture, but if the cell is tilted too steeply then the projected area of the cell in the direction of the incident sunlight becomes small. The maximum tilt angle to consider is the smallest angle such that no photons coming through the aperture are reflected directly back toward the aperture. This maximum tilt angle $\gamma_{max}$ can be given by (see Appendix B for derivation)

$$\gamma_{max} = \psi + \sin^{-1}\left(\frac{r_{cell}}{r_{cav}}\right)$$

where $r_{cell}$ and $r_{cav}$ are the radii of the cell and cavity respectively, and $\psi$ is the aperture acceptance angle. This max angle is not necessarily optimal, as shallower angles resulting in lower cosine losses may outweigh the additional aperture losses. To find an optimum value for the tilt angle, in Fig. 2 we plot the effective absorptance of a cell with an absorptance of 0.5 and varied tilt angle. As expected, effective absorptance increases with tilt angle as aperture losses are reduced until the optimal angle, after which performance degrades due to cosine losses. The maximum tilt angle of 16.5° predicted by Eq. (5) is marked by the dashed vertical line, and in this case the optimal angle is slightly smaller, about 14.5°. It is worth noting that other absorptance values besides 0.5 can be used to optimize the geometric parameters, and the difference in results is negligible for a wide range of absorptances.
Cavity size ratio (the ratio of cavity radius to cell radius) is also important to consider for maximizing cell absorption. Figure 3 shows the fractions of the rays initially reflected from a cell with absorptance of 0.5, which after bouncing within the cavity are (i) absorbed by the cell, (ii) absorbed by the cavity and (iii) lost through the aperture. There is an optimal size ratio, as very small cavities require large apertures to maintain a decent concentration ratio (leading to large aperture losses), while large elliptical cavities focus the rays back out of the aperture in only one reflection off the cell. It can be noted that larger size ratios call for shallower tilt angles and therefore lower cosine losses, an advantage not reflected in Fig. 3. It should also be noted that these results use the tilt angle given by Eq. (5), so slightly improved performance could be obtained by finding the optimal angle at each cavity size ratio.

To calculate how much the cavity enhances the effective absorptance of the embedded PV cell, we fixed the cavity geometry and ran ray tracing simulations for cell absorptances varying from 0 to 1 (Fig. 4b). The cavity parameters used for the results in Fig. 4b (and hereafter) were as follows: an acceptance angle of 5°, a cavity specular reflectance of 95%, a cavity size ratio of 5, and a cell tilt angle of 14.5°. As can be seen in Fig. 4b, the largest enhancements occur for moderate absorptances in the range of ~0.2 – 0.7. The enhancement is small for low cell absorptances because even with additional opportunities for absorbing incident photons, the photons are still more likely to be reflected away from the cell and either escape or get absorbed elsewhere in the cavity. The enhancement is small for high absorptances because almost all the photons are absorbed on the initial incidence on the cell, so there are few additional photons left to absorb with the aid of the cavity. It is also worth noting that for absorptances very close to 1 the cavity actually lowers the cell performance, as the cosine losses from the tilted cell outweigh the advantage of increased absorptance of incident photons.

In order to calculate the absorptance of a PV cell without a cavity, the wave optics module in COMSOL Multiphysics was used to simulate the PV cell optical response including cell reflectance and absorptance for both transverse electric (TE) and transverse magnetic (TM) polarizations. Three types of c-Si PV cell were studied, including unpatterned (planar) thin-film cells and cells with either a three dimensional (3D) pattern of inverted nano-pyramids (INPs) or a two dimensional (2D) pattern of parallel periodic grooves. Silicon nitride antireflection layers with thicknesses of 70 nm and 100 nm were placed on top of the planar and textured silicon layers, respectively. The periodicities for both the 2D grooves and 3D INPs are 700 nm. For textured solar cells, an unavoidable planar area between each repeating unit cell forms a ridge region, which can be seen in Fig. 4a, and this ridge separation is set to be 50 nm[10]. Floquet periodic boundary conditions are implemented on the sides of the computation window, and a perfect electric conductor (PEC) boundary condition is used to mimic the effect of a back mirror for the PV cell. The 2D grooved solar cells have 200nm-thick oxide and 600nm-thick silicon on the back of the silicon. For the 3D inverted pyramids, we assumed a PEC boundary condition directly underneath the silicon layer to improve numerical accuracy and reduce computation time. Absorptance for varying incidence angles from normal to 20° were calculated (capturing the majority of ray incidence angles), however no significant angular dependence was observed in this range.

Since photons absorbed in parts of the cell other than the silicon (e.g., the nitride layer) are not useful, effective absorptance of the cell $A_{eff}$ with the cavity (for a particular wavelength) is given by

$$A_{eff} = \frac{A_{Si}}{A_{tot}} \cdot F(A_{tot})$$

where $A_{Si}$ is the absorptance of the silicon portion of the cell, $A_{tot}$ is the total absorptance of the cell and $F$ is the function which gives the cavity enhancement (i.e., the
cell with the grooved surface, the introduction of the cavity brings performance close to the Yablonovitch limit, while the cell with the inverted nano-pyramids and cavity exceeds the Yablonovitch limit for wavelengths greater than 800 nm. It should be emphasized that photons with the energies in this spectral range close to the bandgap of silicon can be converted most efficiently by Si PV cells. The angle-limited absorption limit is not plotted here (which the proposed cavity would never be able to exceed) as for our cavity’s acceptance angle the absorptance would effectively be unity across the entire spectral range.

To quantify how cavity-enhanced absorptance affects PV cell performance, we calculate the photo-generated current density, $j_{ph}$, and the cell efficiency. Both of these quantities are calculated assuming a solar concentration of 25, chosen because such an optical concentration captures all the sunlight that would be incident on the cavity ($r_{cav}/r_{cell} = 5$). The photogenerated current density can be modeled by assuming that every absorbed photon in the silicon with energy above the bandgap excites one electron-hole pair. The AM1.5D solar spectrum[29] is used, as the cavity-embedded cell is expected to be operated over concentrated sunlight illumination. Efficiency can be calculated using a simple 1D model, with the current density $j$ calculated as:

$$j = j_0 [\exp(qV/kT) - 1] - j_{ph}$$  \hspace{1cm} (7)

where $j_0$ is dark current density, $q$ is elementary charge, $V$ is voltage, $k$ is the Boltzmann constant, and $T$ is cell temperature, with proper silicon properties[30,31]. Efficiencies are calculated assuming p-type cell doping level of $10^{16}$cm$^{-3}$, 500nm-thick n-type junction on the top surface with doping level of $10^{17}$cm$^{-3}$, and surface recombination velocities of 30cm/s at both top and bottom surfaces. Figure 5a shows photo-generated current density and efficiency of planar, grooved, and inverted nano-pyramid (INP) patterned cells with and without the cavity as a function of the cell thickness. The photo-generated current density obtained using the Yablonovitch limit of absorption is shown for comparison.
improvement comparable to that achieved via surface texturing. The trends for the efficiency results, which are shown in Fig 5b, closely mirror what was discussed for photogenerated current.

4. Conclusion

While prior research efforts have focused primarily on surface patterning of solar cells to enhance light trapping, the results reported here show that the proposed optical cavity can also lead to significant absorbance enhancements. This offers an alternative path to improve thin-film PV cell absorbance, which can be pursued either in parallel with surface patterning or separately. Modeling shows that the optical cavity used in conjunction with patterned PV cells can even exceed the Yablonovitch limit for absorption, especially for ultrathin (<2µm) solar cells. The effect of the cavity can be even stronger for thin film PV cells with higher radiative recombination emission rates (such as GaAs), as the cavity-imposed emission angular selectivity also enables recycling of emitted photons[16,21].

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Appendix A – Results showing higher order refractions are negligible

COMSOL simulations can be used to calculate refraction from the surface of a patterned reflector, such as the PV cells investigated in this paper. The reflectance of the 0th, 1st and 2nd order refractions for unpolarized light at a 15° incidence angle on a 10 µm thick cell with a 2D groove pattern is shown in Fig. A1. As can be seen from the plot, the great majority of the contribution to reflectance comes from the 0th order reflection. This was found to be the case for other incidence angles and cell thicknesses as well.

Figure 5 (a) Photo-generated current density and (b) efficiency as a function of cell thickness for planar (red), 2D grooved (green) and 3D INP (blue) surfaces both with (solid curves with pentagrams) and without the cavity (dashed curves with open circles). The photogenerated currents and efficiencies assuming the Yablonovitch limit (dashed black curve) and 2D limit (dotted black curve) for the cell absorptance are shown for comparison.

The photogenerated current density enhancement is most pronounced for planar cells, with improvements of about 7 mA/cm²/sun for very thin cells, and of about 5 mA/cm²/sun for conventional cells with thicknesses of 100µm and above. Planar cells have moderate absorption for a wide range of wavelengths, and thus benefit most from the cavity effect. The enhancement is less dramatic for patterned cells, as they already have fairly good absorptance, however there is still a significant improvement of around 5 mA/cm² for thin cells and 2 – 3 mA/cm² for thicker cells. The enhancement is significant enough that for INP patterned cells of < 2 µm in thickness, the cavity effect pushes the PV photogenerated current above the Yablonovitch limit. The performance of INP patterned cells is only plotted for cells with up to 13 µm thickness due to computational limitations for 3D COMSOL simulations. INP performance is expected to approach grooved cell performance at large thicknesses, as the increased scattering gives diminishing returns for thicker cells, and this trend is already noticeable for the thicknesses shown in Fig. 5. It is also worth noting that the planar cell with the cavity outperforms the grooved cell without the cavity, indicating that use of the cavity as a light trapping strategy achieves PV cell performance

Figure 5 Reflectances for the 0th (solid black curve), 1st (dashed blue curve) and 2nd order (dotted red) diffractions from a 10 µm
thick silicon PV cell at 15° incidence angle as computed by COMSOL

**Appendix B – Derivation of equation (5)**

In order to derive Eq. (5) it is useful to define geometric parameters with respect to the PV cell, as shown in Fig. B1. In this figure, the lines normal to the incident sunlight (dotted green) intersect the lines normal to the PV cell (solid red) at the tilt angle $\gamma$. If the cell is tilted clockwise, the last ray to be captured in the cavity is at the acceptance angle $\psi$ relative to the normal incidence sunlight. This last ray is labeled “A” in Fig. B1. When it reflects from the PV cell, it forms an angle $\gamma - \psi$ relative to the line normal to the PV cell, this reflected ray is labeled “B” and should hit the edge of the aperture. The edge of the aperture is defined by the opposite side of the PV cell, and the line between the edge of the aperture and PV cell (labeled “C”) should be at the acceptance angle $\psi$ relative to the normal incidence sunlight.

Thus, lines from both edges of the PV cell to the edge of the aperture form the same angle with the lines normal to the PV cell: $\gamma - \psi$. This symmetry indicates that this edge of the aperture is at the apex of the hemi-ellipsoidal cavity, at a height of $h$. The distance between the edges of the PV cell and the apex of the dome is given by the Pythagorean theorem as $\sqrt{r_{cell}^2 + h^2}$. By applying Eq. (3), we can see that the distance is simply the semi-major axis of the ellipsoidal cavity $r_{cav}$. This sets up a simple trigonometric equation

$$\sin(\gamma - \psi) = \frac{r_{cell}}{r_{cav}} \tag{B.1}$$

which when rearranged for the tilt angle $\gamma$ yields the form shown in Eq. (5).

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