Light trapping in a 30-nm organic photovoltaic cell for efficient carrier collection and light absorption

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Abstract: We describe surface patterning strategies that permit high photon-collection efficiency together with high carrier-collection efficiency in an ultra-thin planar heterojunction organic photovoltaic cell. Optimized designs reach up to 50% photon collection efficiency in a P3HT layer of only 30 nm, representing a 3- to 5-fold improvement over an unpatterned cell of the same thickness. We compare the enhancement of light confinement in the active layer with an ITO top layer for TE and TM polarized light, and demonstrate that the light absorption can increase by a factor of 2 due to a gap-plasmon mode in the active layer.

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有机光伏（OPVs）具有低成活成本、轻便的太阳能电池技术的潜力，但存在吸收光子和收集光生载流子的权衡。”这种权衡的结果是因为P3HT等活性层的 exciton diffusion length 通常只有 10-15 nanometers 而光吸收长度至少是光的吸收长度的至少一个数量级 [1, 2]。

块异质结设备通过使用光学厚的活性层解决该问题，其间插或投射电极以收集电荷。另一种方法是，我们在此探索的，它使用了光陷阱技术来增强厚度与载流子扩散长度相当的活性层的吸收 [3–9]。

各种技术已经被提出增加光收集，如在活性材料中光子晶格结构 [3, 4] 或在活性层上的金属纳米结构 [5–8]。电介质光栅可以以共振模式的形式限制光，从而增加光吸收在活性层下方。在这种情况下，我们解决光陷阱的方法通过一个详细的数值设计研究一个图案化的顶部电极组成的氧化铟锡（ITO）。在第二段，我们讨论了同时优化两种类型的光限制机制，结果细胞在相关谱范围提供强烈的太阳能吸收。在第3和4段，我们发现这个光带隙模式，它在折射率低的介质中形成OPV吸收介质被ITO和底部金属接触所挟。比较光吸收对于TE和TM偏振光，我们估计光带隙模式在活性区域中导致近2倍的吸收增强。在第5节中，我们将一维的光栅扩展到二维的，从而消除光偏振依赖的吸收增强。使用包含ITO锥的二维光子晶格结构，我们找到有效模式转换从正常方向的太阳辐射到光带隙模式，该模式被金属接触和ITO图案层在顶部所挟。光子晶格图案化结构实现光收集效率40%，代表比无图案结构上的相等吸收层厚度四倍的增强。在第5.2节中，我们发现当ITO圆柱被锥形结构替换时，光收集效率可以增加到50%。在所有情况下，一个持续的ITO层保留在OPV活性材料上以确保高效的载流子收集。
2. Gap-plasmon mode

A gap-plasmon mode (gap mode) is the enhanced confinement of a guided surface plasmon mode at a dielectric-conductor boundary, achieved by introducing a thin layer of low index dielectric material (a gap) between a high-index dielectric cladding and the conductor, and is due to the refractive index change across the dielectric interface. A similar enhancement of the field confinement has been demonstrated in dielectric slot waveguides \[10-12\]. In this case, a dielectric slab waveguide is modified by inserting a low index dielectric layer – the slot – in the middle of the slab; this slot supports a transverse magnetic (TM) mode. If the slot is narrow enough, the profile remains nearly the same as it was in a slab waveguide without the slot, because of the continuity of the electric displacement field,

\[
\varepsilon_w E_w = \varepsilon_s E_s, \quad (1)
\]

\[
\frac{I_s}{I_w} = \frac{|E_s|^2}{|E_w|^2} = \left( \frac{\varepsilon_w}{\varepsilon_s} \right)^2 = \left( \frac{n_w}{n_s} \right)^4. \quad (2)
\]

The subscripts \(w\) and \(s\) stand for the waveguide and the slot, respectively. The intensity of the normal component of the electric field increases by a factor of \((n_w/n_s)^4\) in the slot, resulting in stronger absorption.

Similar to the highly confined guided modes in a dielectric waveguide, enhanced standing surface plasmon modes have been observed in a system composed of a narrow low index gap layer sandwiched between a dielectric waveguide with high index and a metal surface on the other side \[13,14\], and the electromagnetic field can be tightly confined within the gap \[15\]. In this letter, we apply the gap-plasmon mode to the dielectric-gap-conductor structure of the OPV device structure proposed in Fig. 1(a). The periodically patterned dielectric top layer allows for phase matching between incident sunlight and standing surface plasmon gap modes in the P3HT active region for specific wavelengths and angles in regions of the solar spectrum where ITO has a higher index than P3HT. The highly confined gap mode possesses a large in-plane electric field component which leads to a vastly increased optical absorption in the lower index thin film active material.

![Fig. 1. (a) Schematic showing the structure composed of a patterning ITO layer on a 30 nm P3HT absorbing layer. \(h_1\) is the thickness of the ITO Layer, \(h_2\) is the etching depth of the periodic pattern, \(a\) is the period of the pattern, and \(d\) is the width of the ridges. (b) The real part (\(n\)) and the imaginary part (\(k\)) of the refractive index of P3HT (black) and ITO (red).](image-url)
3. 1D grating: rectangular ridges

As illustrated in Fig. 1(a), the first structure considered consists of a 30 nm active layer placed on a reflective metal layer, and a high-index transparent layer imprinted with periodic patterns on the top of the active layer. The material chosen as the active layer is poly-3(hexylthiophene)(P3HT) and we use a perfect electric conductor (PEC) to model the bottom metal electrode in all our numerical calculations. The real \( n \) and imaginary part \( k \) of the refractive index of the material are shown in the black lines in Fig. 1(b), Ref. [16]. We consider the solar spectrum (simulated by a blackbody at 5800 K) from 350 nm to 750 nm, in which P3HT possesses a large absorption coefficient.

To enhance light absorption in the active material, we deposit a transparent layer with high refractive index on the P3HT layer and imprint a one-dimensional pattern of infinitely long square ridges. As defined in Fig. 1(a), the transparent patterned layer has a thickness of \( h_1 \), an etch depth of \( h_2 \), a ridge width of \( d \), and a periodicity of \( a \). We choose ITO as the material of the top layer in the following discussion to satisfy the previously stated criteria and to act as a transparent top electrode for carrier collection in the OPV. The complex refractive index of ITO is shown in the red lines in Fig. 1(b) [17]. According to the difference between the real index of ITO and P3HT, we can separate the wavelength range into two regimes. In the wavelength range of \( \lambda > 520 \text{ nm} \), which we call the resonance regime, the enhancement of the absorption results mainly from the resonance modes induced by the ITO photonic crystal structure. As \( \lambda < 520 \text{ nm} \), the real part of the index of ITO is larger than that of P3HT so that gap modes can be formed in the P3HT layer and contribute to the absorption enhancement. We call this regime the resonance-gap hybrid regime (or, in short, the hybrid regime).

We perform 2D RCWA using the commercially available DiffractMOD simulation package from RSoft Design Group [18] to investigate the dependence of the light absorption in the active layer on all parameters \( h_1, h_2, a, \) and \( d \). For 2D simulations we use 11 Fourier harmonics in the

![Fig. 2. (a) Map of the integrated absorbance \( A \) versus the period of the 1D pattern, \( a \), and the width of the ridges, \( d \), for TE polarized light. (b), (c) The photon collection efficiency spectra of the optimal structure and the unpatterned reference. (d), (e) The intensity distribution of the electric field of the optimized case at wavelengths having maximal and minimal collection efficiency.](image-url)
x-direction, and for 3D simulations we use 11 Fourier harmonics in both the x- and y-direction.

For all numerical calculations, plane waves in free space, with wavelengths from 350 nm to 750 nm, are used to model the incoming solar light, and periodic boundaries are used in the in-plane (x − y) directions. The plane wave source is launched at normal incidence, except for calculations where the angle of incidence is explicitly stated. The figure of merit is defined as

$$A = \int d\lambda \left[ B(\lambda) \frac{P(\lambda)}{hc/\lambda} \right],$$

where $A$ is the total integrated absorbance and $B(\lambda)$ is the collection efficiency of photon, i.e. the calculated fraction of light absorbed in the active layer as a function of wavelength and weighted by the solar irradiance spectrum $P(\lambda)/(hc/\lambda)$, in units of photon flux per unit wavelength. The integral is normalized to unity absorbance.

The absorbance of the planar structure with a 30 nm P3HT layer and no ITO layer is only 10.13%.

3.1. **TE polarized light**

In our investigation of the photon absorption enhancement by the patterned ITO layers, we first focus on the absorption in the active layer for TE polarized light (with only one $E_y$ component). In this case, neither surface plasmon modes nor gap modes exist. In Fig. 2(a), we show the overall photon absorbances of the structure with the optimal $h_1 = 190$ nm and $h_2 = 150$ nm as determined by the numerical simulations, for different combinations of the ridge period, $a$, and ridge width, $d$. A maximum $A = 22.61\%$ occurs at $(a, d) = (560\text{nm}, 100\text{nm})$ (point I). Compared with a structure with an unpatterned top layer (point II, $A = 13.80\%$), the absorbance increases by 64% and its amplitude is more than double that of a structure having only a P3HT layer.

The spectra of the photon collection efficiency of the optimized structure and the unpatterned

![Fig. 3.](image)

Fig. 3. (a) Map of the integrated absorbance $A$ versus the period of the 1D pattern, $a$, and the width of the ridges, $d$, for TM polarized light. (b), (c) The photon collection efficiency spectra of the optimal structure and the unpatterned reference. (d), (e) The intensity distribution of the electric field of the optimized case at wavelengths having maximal and minimal collection efficiency.
reference are shown in Fig. 2(b) and 2(c), respectively. A large peak in the resonance regime with a collection efficiency $B$ of 70% is observed for the optimal case, which agrees with the higher absorbance obtained. Figures 2(d) and 2(e) show the intensity distributions of the electric field along the cross-section of the optimal structure at the peak, $\lambda = 582$ nm, and the nearest local minimum, $\lambda = 750$ nm, respectively. As expected, in both Fig. 2(d) and 2(e), resonance modes induced in the ITO grating are observed, but in Fig. 2(e), there is less intensity distributed in the active layer as the collection efficiency reaches a minimum. This result agrees with the enhancement obtained in a previous study of enhancing light trapping in organic solar cells with dielectric photonic crystal structures as the top-surface layer [9]. Our approach is to apply this result in combination with a gap mode enhancement, so as to achieve a substantially higher absorption enhancement with a smaller active area.

3.2. TM polarized light

As mentioned in Section 2, because the gap mode results from the enhancement of the surface plasmon mode, we can only induce gap modes with TM polarized light (with only one $\vec{H}$ component, $H_y$). As a result, for comparison, we perform a similar calculation for TM polarized light and show, in Fig. 3(a), the impact on the photon absorbance of varying the grating period and the ridge width, using the optimized thickness of the ITO layer and etching depth ($h_1,h_2$)=(200 nm, 170 nm). The optimal structure has $(a,d)$=(440 nm, 190 nm) (Point III) and the calculated overall absorbance is up to 44.36%, which is a factor of 3.4 increased from that of the unpatterned reference (Point IV, $A = 13.17%$). Compared with the optimal value for TE polarized light, which does not involve gap modes, the enhancement of absorbance is doubled, which agrees with our expectation of the contribution of the gap modes. The collection efficiency spectrum shows peaks with collection efficiency $B > 80\%$ in both the resonance and hybrid regimes for the optimal structure (Fig. 3(b)) but not for the unpatterned reference (Fig. 3(c)). Figures 3(d) and 3(e) show the intensity of the electric field of the optimal structure for the peak in the hybrid regime at $\lambda = 364$ nm and the nearest local minimum at $\lambda = 438$ nm. Figure 3(d) shows the clear presence of a gap mode enhancing the absorption in the active layer; only a small residual field is distributed in the active layer in Fig. 3(e).

3.3. Incident-angle dependence

One important property of a solar cell is its tolerance to the angle of the incident light. Figure 4 shows the absorbance of the optimized 1D grating cells for TE and TM polarized light, as a function of incident angle. For TE polarized light, the maximal absorbance occurs when
Fig. 5. (a) Schematic of the ITO grating composed of triangular ridges. (b) The spectral collection efficiencies in the active layer for TE and TM polarized light. (c), (d) The intensities of the electric field for the optimal structure for TE polarized light at $\lambda = 532$ nm and 382 nm, respectively. (e), (f) Electric field profiles for TM polarized light at the same wavelengths.

Fig. 6. Photon absorbance of the triangular ridge structure with optimized geometry versus incident angle, for TE (black line) and TM polarized light (red line), respectively. The dotted lines show the incident-angle dependence of the absorbance for the unpatterned references. Light has normal incidence, and for TM polarized light, the absorbance reaches its maximum, $A = 46.06\%$, when the light is incident with an angle of $4^\circ$ from the vertical and then drops to its $2/3$ as $\phi > 20^\circ$. However, for both polarizations, the absorbance maintains 40% larger than that of the unpatterned reference until the incident angle is up to $80^\circ$. Note that for TM polarized light, the absorbance of the unpatterned reference increases as the incident angle until $\phi > 70^\circ$ because more normal component of electric field can provide stronger gap-plasmon modes in the active layer.
4. 1D grating: triangular ridges

We replace the square-shaped ridges with a triangular shape to achieve better coupling between the normal-incident electric field and the surface plasmon mode. The structure of the solar cell is shown in Fig. 5(a). Figure 5(b) shows the spectral collection efficiency of the optimal structure, which has \( h_1 = 140 \text{ nm}, h_2 = 100 \text{ nm}, a = 520 \text{ nm}, \) and \( d = 130 \text{ nm} \) for TE polarized light, and \( h_1 = 120 \text{ nm}, h_2 = 120 \text{ nm}, a = 360 \text{ nm}, \) and \( d = 290 \text{ nm} \) for TM polarized light. The optimal absorbance is 22.64% for TE polarized light, which is enhanced by a factor of 1.95 from the unpatterned reference (\( A = 11.64\% \)). The optimal absorbance for TM polarized light is 48.73%, which is 10% higher than the optimal value of the rectangular ridges. A total enhancement of 485% over the unpatterned structure is increased by 43%, compared to the 337% enhancement achieved by rectangular-shaped ridges.

Figure 5(c) and 5(d) show the intensity distributions of the electric field for peaks at wavelengths \( \lambda = 532 \text{ nm} \) and \( 382 \text{ nm} \) for TE polarized light. Well-confined resonance modes are observed in the ITO layers. Figure 5(e) and 5(f) show the electric field intensity at the same wavelengths for TM polarized light. Beside the resonance modes, surface plasmon modes are observed near the bottom contact and the gap mode is found in the hybrid regime, both of which contribute to the absorption being two times higher than that for TE light.

Figure 6 shows the incident-angle dependence of the photon absorbance of the optimal triangular-ridge gratings. For TE light (the black line), a maximum exists when the light is normally incident and the absorbance \( A \) remains around 0.2 until the incident angle is larger than 80°. For TM light (the red light), the photon absorbance reaches its maximum value of 52.03%, at \( \phi = 9^\circ \), and decreases to that of the optimal value for TE light when \( \phi < 70^\circ \).
5. 2D gratings

5.1. Cylinder and block arrays

To account for the randomly polarized nature of sunlight, we extend the pattern structure from 1D to 2D in order to eliminate the polarization dependence of the absorption enhancement. Figure 7(a) shows the structure of the 2D patterns that are composed of ITO cylinders and blocks in square lattices. The optimal structure of the cylinder array has $h_1 = 250$ nm, $h_2 = 220$ nm, $a = 460$ nm, the diameter of the cylinders, $d = 260$ nm, and the absorbance is 40.89%. The optimal block array has the same $h_1$, $h_2$, and $a$ but a different block width, $d$, of 240 nm, and the absorbance is 40.55%. In both cases, the light absorbance is enhanced by a factor of $\approx 3.4$ over that of an unpatterned ITO layer.

As expected, the cylinder array provides stronger confinement of light than the block array because circular arrays have higher symmetry; however, the absorption enhancement remains almost the same for both structures. We compare the absorption spectra, $B(\lambda)$, of the optimal cylinder and block arrays in Fig. 7(b). Peaks with high collection efficiency are observed in or near the resonance regime at similar wavelengths for both structures. The peak at $\lambda = 670$ nm red shifts for the block array due to the higher effective refractive index. We also observe that a peak exists for the block geometry, but not for the cylinder geometry, in the hybrid regime at $\lambda = 370$ nm, where the difference between the index of ITO and P3HT is sufficiently large to support a gap mode. In comparing the intensities of the electric field for the cylinder array at $\lambda = 370$ nm in Fig. 7(c) with that of the block array in Fig. 7(e), it can be seen that for the cylinder array, the resonance mode of the grating is better confined, but the block array can better couple to gap modes in the active layer because of its less symmetric shape in the in-plane direction, which agrees with the higher collection efficiency obtained.

5.2. Cone arrays

We perform numerical simulations for a 2D grating composed of cones in a square lattice with a similar motivation to the 1D triangular gratings. The optimal structure of the cone array has the dimensions of $h_1 = h_2 = 160$ nm, and $a = d = 430$ nm, and the optimal photon absorbance is 49.46%, which is enhanced by a factor of 3.7 from that of the unpatterned reference ($\alpha = 13.33\%$). Compared with cylinder or block arrays, the photon absorbance is 25% higher and the enhancement over the unpatterned reference increases by 9%. Figure 8(c) shows the intensity...
distribution of the electric field for a collection efficiency peak exceeding 80% at $\lambda = 444$ nm, which is in the hybrid regime. As can be seen, a gap mode is formed, accompanied with a strongly confined resonance mode in the grating.

5.3. Incident-angle dependence

Figures 9 shows the incident angle dependence of the absorbance for the optimal cylinder, block, and cone arrays. The absorbance values of the 2D arrays reach the maxima at $\phi = 6 - 12^\circ$ and are about 5 – 11% higher than those with normal incident light. The maximal absorbance for the cone array can be up to $A = 55.12\%$ when light is incident at an azimuth angle of $9^\circ$ along the lattice, and $A = 55.80\%$ at $\phi = 12^\circ$ along the diagonal. For all structures, the photon absorbance remains greater than 50% higher than for the unpatterned reference, until $\phi > 70^\circ$. Similar to the 1D cases, the absorbance of unpatterned references increase with the incident angle until $\phi > 75^\circ$.

6. Conclusion

We have extensively studied how different patterning geometries on the top surface of an top-surface ITO contact can effect photon absorption enhancement in an ultra-thin OPV cell. We demonstrate that, in comparison with the enhancement contributed by the resonance modes of a grating only, the enhancement of the photon absorption can be doubled by decreasing the thickness of the active layer to enable gap modes. The photon absorbance can be enhanced by a factor of 3.7 to $\approx 50\%$ for the optimal 2D cone array, and all types of cells possess large incident-angle tolerance (for angles of $> 70^\circ$). This result represents a potential major improvement in optical harvest efficiency for OPVs. We believe this technique can thus lead to a substantial advance in the efficiency of organic solar cells, which has previously been limited by the mismatch between the exciton diffusion length and the absorption length.

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