Light trapping beyond the $4n^2$ limit in thin waveguides

Jeremy N. Munday,[1,2,a)] Dennis M. Callahan,[2] and Harry A. Atwater[2]
[1]*Department of Electrical and Computer Engineering and the Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, Maryland 20742, USA*
[2]*Thomas J. Watson Laboratories of Applied Physics, California Institute of Technology, Pasadena, California 91125, USA*

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We describe a method for determining the maximum absorption enhancement in thin film waveguides based on optical dispersion relations. For thin film structures that support one, well-confined guided mode, we find that the absorption enhancement can surpass the traditional limit of $4n^2$ when the propagation constant is large and/or the modal group velocity is small compared to the bulk value. We use this relationship as a guide to predicting structures that can exceed the $4n^2$ light trapping limit, such as plasmonic and slot waveguides. Finally, we calculate the overall absorption for both single and multimode waveguides, and show examples of absorption enhancements in excess of $4n^2$ for both cases. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.3695156]

The confinement of light in thin waveguides is of great importance for the development of thin film photovoltaics. When the thickness of the film is less than the absorption depth of the material, not all of the incident light can be absorbed on a single or double pass through the absorber. However, a thin film is sometimes necessary to allow for efficient collection of carriers or to improve the cell's performance based on reducing the cell's recombination current.[1] For weakly absorbing materials whose thickness h is significantly larger than the wavelength of the incident light λ, the path length enhancement is given by $4n^2$, where n is the index of refraction of the absorber.[2,3] An extension of this method, which is based on a statistical distribution of the electromagnetic energy density, to the case where $h \sim \lambda$, was performed by Stuart and Hall.[4] By considering the reduction in the number of photonic modes in an absorbing slab as the slab's thickness is reduced, they concluded that the maximum absorption enhancement is reduced below $4n^2$.

Despite the early work suggesting that the absorption enhancement in thin slabs is less than $4n^2$, recent work has shown that the enhancement may in fact exceed this limit through the use of photonic crystals,[5] plasmonic waveguides,[6] and high index claddings,[7,8] which all elevate the local density of optical states to achieve enhancment.[9] Here we revisit the case of a thin waveguide and determine that the $4n^2$ limit can be exceeded for a number of structures that support large propagation constants and/or slow modal group velocities.

We follow a formalism similar to Refs. 4 and 6 and begin by considering the thermal occupation of electromagnetic modes in a waveguide surrounded by vacuum. The total density of modes per unit volume and frequency is given by,[4]

$$\rho_{tot} = \rho_{rad} + \sum_m \rho_m \tag{1}$$

where

$$\rho_{rad} = \left(1 - \sqrt{1 - 1/n_{sc}^2}\right)\left(\frac{\omega^2 n_{sc}^3}{\pi^2 c^3}\right). \tag{2}$$

is the density of radiation modes not trapped by total internal reflection within a material of index n_{sc}, and

$$\rho_m = \frac{\beta_m}{2\pi h v_g^m} \tag{3}$$

is the density of waveguide modes with modal propagation constants β_m and group velocities v_g^m for the mth mode. Assuming that the modes of the structure are equally occupied from an appropriate incoupler, the total fraction of incident light absorbed by the film is[6]

$$F_{tot} = \frac{\rho_{rad}}{\rho_{tot}} f_{rad} + \sum_m \frac{\rho_m}{\rho_{tot}} f_m, \tag{4}$$

where

$$f_{rad} = \alpha \Bigg/ \left(\alpha + \left[4\left(\frac{\rho_{tot} v_g^{rad}}{\rho_0 v_g^0}\right) h\right]^{-1}\right) \tag{5}$$

and

$$f_m = \alpha\Gamma_m \Bigg/ \left(\alpha\Gamma_m + \left[4\left(\frac{\rho_{tot} v_g^{rad}}{\rho_0 v_g^0}\right) h\right]^{-1}\right). \tag{6}$$

α is the attenuation coefficient, Γ_m is modal confinement factor, $\rho_0 = \omega^2/(\pi^2 c^3)$ is the bulk density of states in vacuum, and $v_g^0 = c$ is the speed of light in the surrounding vacuum. In Eq. (4), note that the ratios of the density of states gives the fraction of light that enters each mode and f_{rad} and f_m give the rate of absorption divided by the total rate of energy loss (absorption and out coupling).

a)Author to whom correspondence should be addressed. Electronic mail: jnmunday@umd.edu.

We now consider the case of a thin waveguide that only supports one guided mode. For this case $\rho_{rad} \ll \rho_m$, and the total fraction of light absorbed can be approximated by

$$F_{1-\mathrm{mode}} = \alpha\Gamma_m \Big/ \left(\alpha\Gamma_m + \left[4\left(\frac{\rho_m \mathrm{v}_g^{rad}}{\rho_0 \mathrm{v}_g^0}\right)h\right]^{-1}\right)$$
$$= \alpha\Gamma_m \Big/ \left(\alpha\Gamma_m + \left[4\left(\frac{\beta_m \pi c^3}{2\omega^2 h \mathrm{v}_g^m n_{sc}}\right)h\right]^{-1}\right), \quad (7)$$

which can be compared to the fraction of light absorbed in the traditional $4n^2$ limit,[10]

$$F_{4n^2} = \alpha \Big/ \left(\alpha + [4n_{sc}^2 h]^{-1}\right). \quad (8)$$

In order to exceed the $4n^2$ limit, $F_{1\text{-mode}}$ must be greater than F_{4n^2}. With the condition $F_{1-\mathrm{mode}} > F_{4n^2}$, we obtain our central result,

$$\left(\frac{\beta_m}{k_0}\right)\left(\frac{\mathrm{v}_g^{rad}}{\mathrm{v}_g^m}\right)\Gamma_m > 4n_{sc}\left(\frac{h}{\lambda}\right). \quad (9)$$

Thus in order to surpass the $4n^2$ limit, we want well-confined modes ($\Gamma_m \sim 1$) that have large propagation constants ($\beta_m > \mathrm{k}_0$), small group velocities ($\mathrm{v}_g^m < \mathrm{v}_g^{rad}$), and waveguide thicknesses that are small compared to the wavelength of the incident light. By comparing Eqs. (7) and (8), we note that the path length enhancement l_{path} is

$$l_{path} = \left(\frac{c}{v_g^m}\right)\left(\frac{\beta_m}{k_0}\right)\left(\frac{\lambda}{h}\right)\Gamma_m. \quad (10)$$

The actual path length is $l_{path}\ h$ for the single mode waveguide case compared to $4n^2 h$ for the traditional limit.

For a given waveguide structure, the dispersion relation is calculated to determine the modal parameters needed for Eq. (9). Figure 1 shows the dispersion relation for several structures based on a thin film of P3HT:PCBM, a common polymer solar cell blend.[11] The propagation constants are obtained from the x-axis, and the slopes of the curves are proportional to the group velocities. Traditional photonic modes for the slab are confined to the region between the vacuum light line and the absorber light line (light blue region). In this region, $\beta_m < \mathrm{k}_0$, $\mathrm{v}_g^m > \mathrm{v}_g^{rad}$, and $\Gamma_m \ll 1$ when the waveguide is thin. Thus, these photonic slab modes cannot surpass the $4n^2$ limit, which is the conclusion reached by Stuart and Hall as they considered only modes in this region.[4]

Figure 1 also shows the dispersion relation for three structures that have large β_m, slow v_g^m, and large confinement factors. These structures include a surface plasmon polariton waveguide, a high-low-high index dielectric slot waveguide, and a metal-insulator-metal (MIM) waveguide. These dispersion curves represent the lowest order TM modes for the structures; however, higher order modes may exist depending on the thickness of the slab. While Eq. (9) is strictly valid only for a single, highly confined mode, the behavior of the

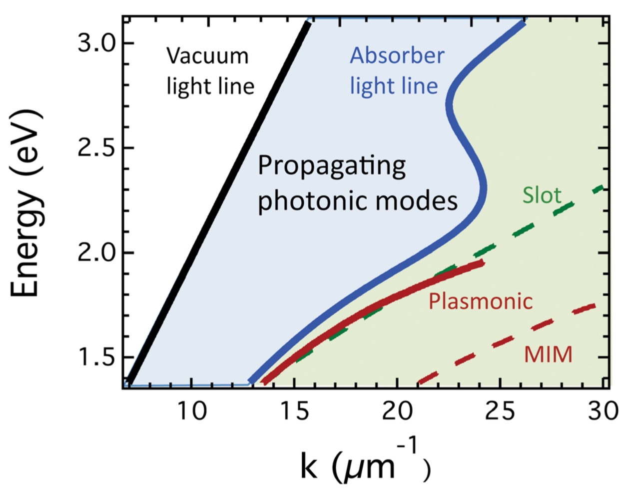

FIG. 1. (Color online) Waveguide dispersion relations. Plasmonic (solid red), metal-insulator-metal (dashed red), and high-low-high index dielectric slot (dashed green) waveguides have dispersion relations that lie to the right of the bulk absorber light line (solid blue), which have large propagation constants, slow group velocities, and are well-confined.

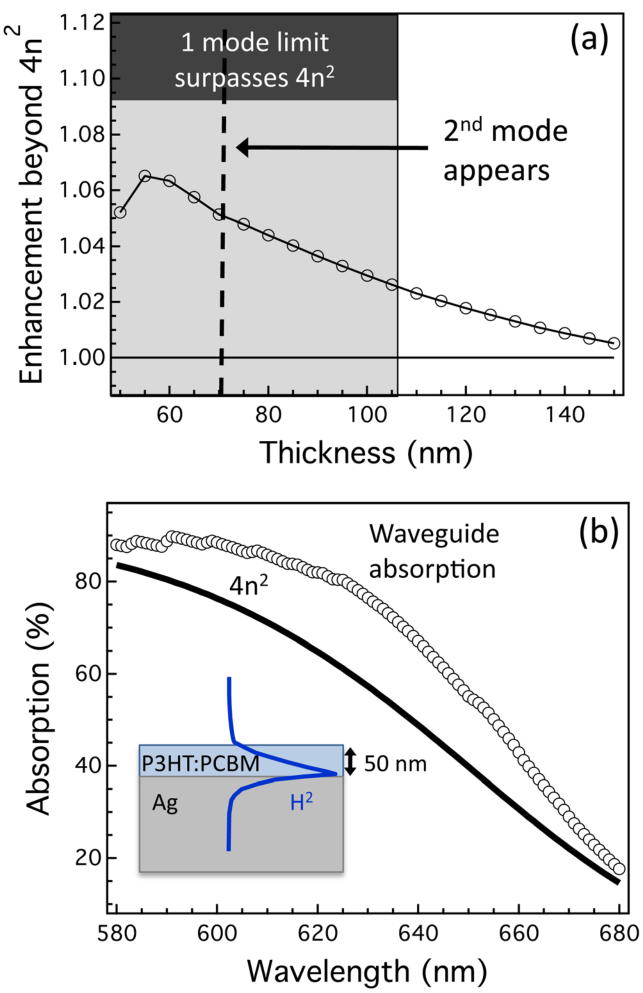

FIG. 2. (Color online) Surface plasmon polariton waveguides that beat the $4n^2$ limit. (a) Calculated absorption enhancement (for $\lambda = 580$ nm) surpasses the $4n^2$ limit for a large range of thicknesses. The shaded region corresponds to the region where the limit is surpassed if only one mode were present. The appearance of a second mode (vertical dashed line) allows the absorption to surpass the $4n^2$ limit beyond the region predicted by the single mode model. (b) Plasmonic waveguide absorption surpasses the $4n^2$ limit throughout the useful absorbing spectrum of the polymer. Inset: Schematic of the plasmonic waveguide and the modal profile.

fundamental mode is often a good indicator of the overall absorption characteristics, as we shall see below.

A thin surface plasmon polariton waveguide (Fig. 2) satisfies the necessary conditions to surpass the $4n^2$ limit for a variety of wavelengths and slab thicknesses. Using Eq. (9), we find that the path length enhancement should exceed $4n^2$ for absorber thicknesses between 50–105 nm (shaded region). However, the condition of only one well-confined mode in the structure is not met for thicknesses larger than 70 nm, because a second mode exists for larger slab thicknesses. Further, below 50 nm, the confinement factor is reduced. Figure 2(a) shows the actual absorption enhancement beyond $4n^2$ (circles) for $\lambda = 580$ nm using Eq. (4), which takes into account both propagating and radiation modes. This structure surpasses the $4n^2$ limit for the entire range. The wavelength resolved absorption for a 50 nm thick slab of P3HT:PCBM on Ag is shown in Fig. 2(b).

A high-low-high index dielectric slot waveguide is also found to exceed the $4n^2$ limit. This structure consists of a 10 nm P3HT:PCBM layer cladded on both sides by a 45 nm layer of GaP, a wide bandgap semiconductor with an indirect energy gap whose absorption is negligible over the wavelength region of consideration and whose real part of the refractive index exceeds that of P3HT:PCBM. This structure supports multiple modes; however, we can use our expression for the path length enhancement to predict whether or not the structure could surpass the $4n^2$ limit if only one mode were present. Figure 3(a) shows that the lowest order TE and TM modes for $\lambda = 580$ nm would both have path length enhancements in excess of $4n^2$ if this were a single mode waveguide.

Figure 3(b) shows the total absorption in the slot waveguide and the fraction of absorption coming from each of the modes. For wavelengths below 620 nm, there are three propagating modes; however, for longer wavelengths, there are only two modes because the second order TE mode is cut off. Because the cladding layer is thin, the radiation modes were assumed to be incident from vacuum and resulted in < 1% of the total absorption. If the radiation modes were allowed to occupy the full 4π steradians, ρ_{rad} would still contribute to less than 3% of the total absorption. Thus the main contribution to the absorption comes from the propagating waveguide modes. We note that the absorption in this high-low-high index dielectric slot waveguide is in excellent agreement with the calculated absorption using the local density of optical states, as recently shown in Ref. 9. A key new feature of using the dispersion relations is that we can now determine the individual contributions of each waveguide mode. We find that both the fundamental TE and TM modes give nearly equal contributions to the enhancement for this structure.

Finally, we explore a hybrid waveguide that combines the benefits of both a high index cladding and a plasmonic back reflector to achieve over 90% absorption in a 10 nm P3HT:PCBM layer—well in excess of the $4n^2$ limit for P3HT:PCBM. The high index GaP cladding further confines the mode and reduces its group velocity. Figure 4 shows the total waveguide absorption, the absorption expected for $4n^2$ passes, and the absorption obtained by a 10 nm thick

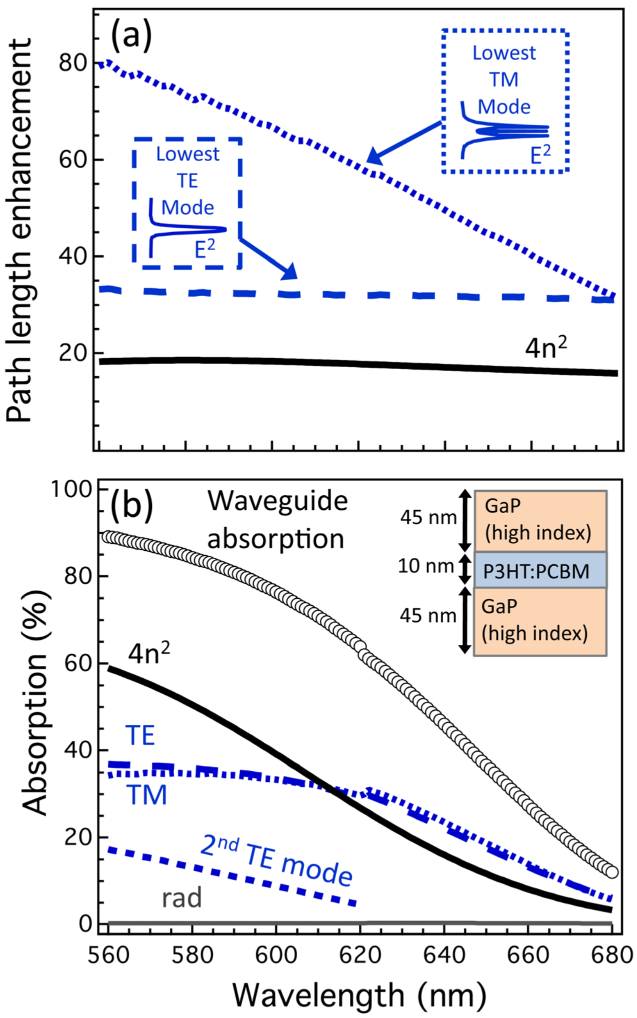

FIG. 3. (Color online) Dielectric slot waveguide that beats the $4n^2$ limit. (a) Path length enhancement if only one mode were present. Both the lowest TM and TE modes surpass $4n^2$. Insets: Mode profiles. (b) Modal decomposition of the absorbed fraction of the incident light. The total absorption surpasses the $4n^2$ limit. Inset: Schematic of the high-low-high index dielectric slot waveguide.

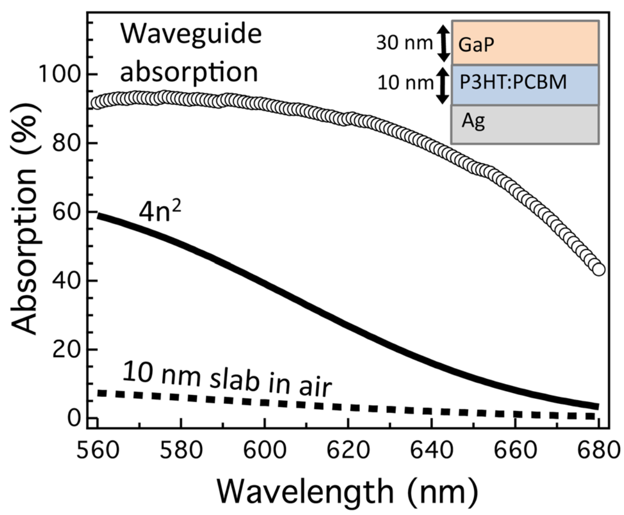

FIG. 4. (Color online) Absorption for a plasmonic waveguide cladded with a high index (GaP) top layer. Waveguide absorption (circles) is well in excess of the $4n^2$ limit (solid line) and the calculated absorption limit for a planar slab in vacuum (dashed line).

P3HT:PCBM film surrounded by vacuum. Note that the 10 nm thick P3HT:PCBM film in vacuum has a significantly lower absorption than would be expected by the $4n^2$ limit. This is due to the fact that the photonic modes are not well confined, have higher group velocities than do modes in the bulk, and have small propagation constants, which are in agreement with the conclusions of Ref. 4.

In summary, we have described a general method for predicting whether or not thin waveguides can have absorption enhancements in excess of the $4n^2$ limit based on their dispersion relations. We gave several examples of such structures by including plasmonic back reflectors and/or high index claddings in order to manipulate the modal propagation constant, group velocity, and confinement factor. Our results are in agreement with recent studies that calculate the local density of optical states[9]; however, the method presented here allows us to resolve the contributions of the individual waveguide modes, which can be enhanced further through appropriate waveguide dispersion engineering. Thus, our results provide both a qualitative and quantitative design scheme for improving the light trapping in thin films, which is highly desired for solar cell applications.

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