Inverse design optimization for efficient coupling of an electrically injected optical antenna-LED to a single-mode waveguide

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Abstract: Efficient high-speed nanoscale optical sources are required for low-power next-generation data communication. Here we propose an integrated antenna-LED on a single-mode optical waveguide. By leveraging inverse design optimization, we achieved a waveguide coupling efficiency of 94% and an antenna efficiency of 64%, while maintaining a high average enhancement of 144 – potentially enabling >100GHz direct modulation.

1. Introduction

The development of high-density integrated optical interconnects is increasingly important to reduce on-chip energy consumption to less than 10fJ/bit [1]. Integrated optical interconnects require fast and efficient nanoscale light sources that are electrically injected and capable of being efficiently coupled to a photonic waveguide. While lasers are extensively used for efficient high speed optical communication, shrinking them down to the nanoscale poses significant problems due to metal loss [2]. LEDs are capable of scaling down to the nanoscale and can operate efficiently without a threshold, but they are limited in speed by their spontaneous emission rate to about 1GHz. However, by coupling the LED to an optical cavity, we can enhance the spontaneous emission rate [3–7], which would allow for >100GHz direct modulation. Only a few reports have demonstrated electrical injection [7–9], with the electrically injected cavity-backed slot antenna (Fig. 1) demonstrating ~200x peak enhancement [7].

As shown in Fig. 1(b), the radiation of the cavity-backed slot antenna is primarily directed towards the substrate, making it a non-trivial problem to couple to a photonic waveguide. Many methods have been used to couple nanoscale devices to waveguides, including coupling an optically pumped dipole antenna to a multimode waveguide using the waveguide height to cancel the electric field propagating toward the substrate [10], an electrically injected metal cavity LED and laser on a single-mode waveguide using the mode shape in the metal cavity [11,12], and using anti-symmetric second-order resonance for a double nanogap plasmonic antenna [13]. Overall, efficient devices that are compatible with electrical injection and have high enhancement are still needed.

Electromagnetic inverse design has been used to improve characteristics of a multitude of photonic devices [14–22]. Inverse design methods allow one to efficiently find non-intuitive geometric structures that optimize electromagnetic figures of merit. For example, inverse design has been used to find high efficiency vertical grating couplers [14], to design a small footprint polarization beamsplitter [15], to optimize a broadband two-mode de-multiplexer [16], to increase the near-field enhancement of an optical antenna while minimizing temperature rise [17], and to optimize fabrication-constrained silicon photonic devices [18].
In this report, we designed and simulated various waveguide coupled antenna-LEDs. We then used inverse design optimization on our best hand-designed structure to generate two structures optimized at a single frequency and multiple frequencies, respectively. In our multi frequency design, we achieved a waveguide coupling efficiency of 94%, an antenna efficiency of 64%, and an average enhancement of 144. The proposed design is potentially compatible with electrical injection and top down fabrication.

![Diagram of antenna-LED structure](image)

**Fig. 1.** (a) Vertical cross section schematic and (b) power flow of optical antenna-LED on a bulk InP substrate. The XZ cross section depicts the LED length and height.

### 2. Design background

#### 2.1. Cavity-backed slot antenna on a bulk InP substrate

The cavity-backed slot antenna is a promising candidate as an optical source due to its high spontaneous emission enhancement and compatibility for top down fabrication and electrical injection [7]. As shown in Fig. 1(a), the cavity-backed slot antenna is self-aligned to an InP/InGaAs/InP ridge (length: ~130nm, width: 20nm, height: 140nm), where the height and length were chosen to tune the resonance frequency to best match the LED material spectrum, while maximizing the radiated power for the fundamental antenna mode. The antenna is electrically connected to the top of the ridge, where it is used as a contact to inject electrons into the n-InGaAs contact layer. The holes are injected into the p-InP layer, which is insulated from the antenna using a 40nm thick spin on glass (SOG). Finally, the InGaAs quantum well active region is electrically insulated from the antenna using a 1nm thick Al₂O₃ surrounding the ridge sidewalls. When an electron and hole recombine in the active region it acts as a dipole excitation of the antenna mode. In our 3D finite-difference time-domain (FDTD) simulations, we excited the antenna by placing an electric dipole source in the active region.

#### 2.2. Figures of merit

The presence of the optical antenna causes the dipole to radiate more power than if it was in bulk InGaAs, the ratio of these powers provides the enhancement spectrum [3]. For a fair analysis we considered all the dipoles in the active region, accounting for polarization, position, and overlap with the material spectrum. This gives the average enhancement ($F_{\text{avg}}$), which is directly related to both the output power and the modulation rate.

In addition to the average enhancement, we considered the average antenna efficiency ($\eta_{\text{antenna}}$) and waveguide coupling efficiency to the fundamental mode ($\eta_{\text{WC}}$). The antenna efficiency is the fraction of total optical power which is not lost to metal (i.e. the power that reaches the far field). The waveguide coupling efficiency is the fraction of the far field power in the fundamental mode of the waveguide (i.e. it only accounts for the scattering loss). For explicit definitions and averaging factors used see *Appendix: Figures of merit*. In the remainder of the text the figures of merit discussed are these average quantities, unless otherwise noted.
Fig. 2. Cross section, power flow, and waveguide coupling efficiency to the fundamental mode ($\eta_{WC}$) for (a) antenna-LED on single-mode InP waveguide and SiO$_2$ ridge, (b) antenna-LED on single-mode InP waveguide with metal wrapped around waveguide facet, and (c) antenna-LED on single-mode InP tapered waveguide with metal wrapped around waveguide facet and sidewalls (see Fig. 3(a) for perspective view, Fig. 4(b) for top view cross section). See Appendix: Field profiles for the $E_x$ and $E_y$ field profiles of the mode in the InP waveguide.
2.3. Waveguide coupling design

In our previous work we proposed designs to couple light from the cavity-backed slot antenna to a single-mode waveguide [23, 24]. In this subsection we will describe some of the intuition behind these designs, and how they helped achieve efficient waveguide coupling. As shown in Fig. 2(a), we optimized the waveguide height and width in order to cancel the fields propagating towards the substrate (similar to [10]) and achieved a waveguide coupling efficiency of 24% in each direction with a waveguide height of 180nm and a width of 550nm. In Fig. 2(b), we truncated the waveguide and wrapped metal around the end of the facet to effectively act as a mirror. In addition to making the coupling unidirectional, the mirror created an image dipole \(180^\circ\) out of phase with the antenna-LED, which further suppressed fields propagating toward the substrate. By minimizing the separation between the antenna-LED and the back mirror, we achieved a waveguide coupling efficiency of 74% – note this was more than double the result from Fig. 2(a). Finally, in Fig. 2(c) we improved the coupling to the fundamental mode by tapering the waveguide near the antenna-LED and wrapping metal around the sidewall of the tapered section. Figure 3(a) shows the perspective view and Fig. 3(b) shows the enhancement, antenna efficiency, and waveguide coupling efficiency spectra. With this structure we were able to achieve an average enhancement of 162, a waveguide coupling efficiency of 90\%, and an antenna efficiency of 49\%.

![Diagram](image.png)

**Fig. 3.** (a) Perspective view of tapered waveguide coupler with a waveguide height of 180nm and width of 550nm on a 500nm tall SiO\(_2\) ridge, and (b) enhancement, antenna efficiency, and waveguide coupling efficiency spectra.
Although our hand-optimized results are comparable to the best results in the literature, we were restricted to exploring only simple geometries of the waveguide coupler due to the immense computational resource requirements of simulating fine-meshed three-dimensional optical structures. In order to more completely explore the parameter space associated with this waveguide coupler, we applied computational inverse design techniques.

3. Inverse design

Gradient-descent based optimization using the adjoint method can be used to optimize almost any user-defined electromagnetic figure of merit over an arbitrarily large parameter space with minimal computational resource requirements [19,20]. In the literature this optimization method and similar topology optimization methods are commonly referred to by the more general term inverse design, which we will adopt in order to help easily distinguish the various results in this report. For brevity we will not delve into the details of the method, but we recommend the reader review the works in [18–22] for more information. See Appendix: Inverse design for specifics regarding our implementation of inverse design.

Fig. 4. (a) Cross section schematic (XZ) of tapered waveguide coupler showing dashed cutline, and (b) top view XY cross section of waveguide along dashed cutline. (c) XY cross section of coupler after optimization, showing perturbations to Ag-InP boundary. Note (b) and (c) also show the projection of the LED base.
Inverse design was applied to the 2D cross section of the tapered coupler (Fig. 4(b)) to optimize enhancement, antenna efficiency, and waveguide coupling efficiency by perturbing the interface between InP and Ag (Fig. 4(c)) – the spectra before optimization are shown in Fig. 3(b). Our initial inverse design cost function was the power transmitted through the waveguide at a single frequency (spectral product at the resonant frequency of enhancement, antenna efficiency, and waveguide coupling efficiency). This led to a slight improvement in the power transmitted at resonance compared to the tapered coupler – shown in Fig. 5(a) and Fig. 3(b), respectively. However, when calculating the average values, we noticed there was a large trade-off between average enhancement and antenna efficiency. When compared to the tapered coupler, even though the peak enhancement increased from 1034 to 1312, the average enhancement only increased from 162 to 164. However, the antenna efficiency dropped from 49% to 40%. Waveguide coupling increased slightly from 90% to 94%. When we combine these numbers, we see that the average power of the single frequency optimization was lower than the tapered coupler. This is not surprising since the cost function did not represent an average value.

![Inverse Design: Single Frequency](image1)

![Inverse Design: Multi Frequency](image2)

Fig. 5. Enhancement, antenna efficiency, waveguide coupling efficiency spectra and top view XY cross sections for (a) single frequency optimization and (b) multi frequency optimization. For reference, the LED material spectrum \( L(\omega) \) between its 50% power points is shown by the gray shaded region.
In order to increase the average power transmitted, we changed the inverse design cost function to be the weighted sum of the optical power at three frequencies. We weighted the power transmitted at resonance ten times less than the power transmitted at \( \pm 55 \text{THz} \) (\( \pm 40 \text{nm} \)) from resonance to encourage a broader enhancement spectrum. As shown in Fig. 5(b), we were able to create a broader enhancement spectrum with a greater antenna efficiency – ultimately achieving \( F_{\text{avg}} = 144 \) and \( \eta_{\text{antenna}} = 64\% \).

4. Discussion

Our design methodology is contingent on the LED material spectrum, shown in the Appendix, Fig. 7. Given a narrower material spectrum, the single frequency design could be more desirable since the average enhancement would be much larger than the multi frequency design or tapered coupler. Even with our current material spectrum, the single frequency design will theoretically have the fastest direct modulation rate – however at a great expense to antenna efficiency. In contrast, the multi frequency design will have a slower direct modulation rate, but it maintains high enhancement while achieving the highest efficiency making it capable of delivering the most optical power to the waveguide. In fact, when we compare the product of \( F_{\text{avg}}, \eta_{\text{antenna}}, \) and \( \eta_{\text{WC}} \) from the multi frequency design with the cavity-backed slot antenna on a bulk InP substrate, we find that we could emit slightly more power in the fundamental mode of an InP waveguide than would be radiated in all directions for the bulk InP substrate case.

Close observation of the multi frequency design enhancement spectrum in Fig. 5(b) reveals two distinct peaks. This can be explained by thinking of the antenna-LED and coupler section (see inset Fig. 6(a)) as coupled resonators. When they have the same resonance frequency, it will lead to a frequency split that can be observed in the enhancement spectra. This was confirmed by sweeping the LED length in the multi frequency design, which resulted in an avoided crossing between the antenna-LED resonance and the coupler section resonance, as shown in Fig. 6. The dashed black line was generated by sweeping the length of the antenna-LED on a bulk InP substrate (Fig. 1(a)). The dashed green line was created by placing a dipole in the coupler section (see inset) and sweeping the length of an off-resonance antenna-LED. During the length sweep we found that the antenna efficiency always peaked at the coupler section resonance rather than at the antenna-LED resonance.

![Fig. 6](image-url)
A similar observation was made in the single frequency design in Fig. 5(a), the antenna efficiency peak was associated with the coupler resonance. However, in contrast to the multi frequency design, the antenna-LED and coupler section resonances are detuned – evident by the offset between the peak enhancement and antenna efficiency wavelengths in Fig. 5(a).

To summarize, the spectra of the waveguide coupling designs can be explained by considering the antenna-LED and the coupler section as coupled resonators. When the resonances are tuned (multi frequency design), we have an impedance match and frequency splitting. Due to the impedance match, the optical power is able to quickly leave the lossy antenna-LED (lower Q factor) resulting in less metal loss (higher antenna efficiency). In contrast, when the resonances are detuned (single frequency design), we have an impedance mismatch which results in the optical power reflecting back to the lossy antenna region. This results in more metal loss (lower antenna efficiency) and higher enhancement. A similar conclusion was reached in [25], where detuned resonators were exploited to achieve higher peak enhancement. Note that regardless of how the coupler section resonance was tuned, both these designs yielded higher waveguide coupling efficiency than the tapered coupler.

5. Conclusion

We have demonstrated that the cavity-backed slot antenna-LED can be efficiently coupled to a single-mode waveguide, which was validated using relevant figures of merit in an optical interconnect. Then, using inverse design we further optimized the cavity-backed slot antenna coupling, ultimately achieving a waveguide coupling efficiency of 94%, antenna efficiency of 64%, while maintaining a high average enhancement of 144. We found that inverse design was able to achieve these results by tuning the optical resonance of the coupler section relative to the antenna-LED based on our cost function.

Due to its high efficiency, nanoscale size, compatibility with top-down fabrication, and speed the cavity-backed slot antenna-LED is a very promising transmitter for an on-chip optical interconnect.

Appendix

Figures of merit

In Fig. 7, we show the FDTD simulation of the enhancement spectrum of a dipole source with the optimal polarization and position in the cavity-backed slot antenna on a bulk InP substrate from Fig. 1(a). Additionally, the experimental material spectrum from a large area LED with the same epitaxial layers as Fig. 1(a) is provided by the dashed black line in Fig. 7. The product of the material spectrum and the enhancement spectrum gives the output power spectrum from the dipole source.

In order to calculate the average increase in output power (i.e. the average enhancement) we need to account for all the dipoles in the active region. Therefore, we consider the dipole frequency response, polarization dependence, and position dependence. We defined the average enhancement as the following:

\[
F_{\text{avg}} = \frac{1}{2} \times 0.79 \times \frac{\int F(\omega)L(\omega)d\omega}{\int L(\omega)d\omega}
\]  

(1)

where \( \frac{1}{2} \) is the polarization average, 0.79 is the spatial average, \( F(\omega) \) is the overall enhancement spectrum seen by a dipole with the optimal polarization and position, and \( L(\omega) \) is the experimental material spectrum without an antenna present. Note that the final term in Eq. (1) is the spectral average. In principle the material spectrum \( L(\omega) \) is dependent on the carrier concentration; however, in this report we fixed \( L(\omega) \), and therefore the carrier concentration in order to simplify
Fig. 7. Dashed black and solid red lines show the experimental non-enhanced material spectrum \([L(\omega)]\) and the simulated enhancement spectrum \([F(\omega)]\) of the cavity-backed slot antenna on a bulk InP substrate, respectively.

The spatial average and polarization average were found by sweeping dipole position and polarization in the quantum well active region in the cavity-backed slot antenna.

In addition to the average enhancement, we considered the antenna efficiency (\(\eta_{\text{antenna}}\)) and waveguide coupling efficiency to the fundamental mode (\(\eta_{\text{WC}}\)). The antenna efficiency only accounts for the metal loss, and the waveguide coupling efficiency only accounts for the scattering loss. The explicit definitions for the antenna efficiency and waveguide coupling efficiency spectra are shown below:

\[
\eta_{\text{antenna}}(\omega) = \frac{P_{\text{total}}(\omega) - P_{\text{metal loss}}(\omega)}{P_{\text{total}}(\omega)} \tag{2}
\]

\[
\eta_{\text{WC}}(\omega) = \frac{1}{\eta_{\text{antenna}}(\omega)} \frac{P_{\text{fundamental mode}}(\omega)}{P_{\text{total}}(\omega)} \tag{3}
\]

\[
P_{\text{total}}(\omega) = P_{\text{fundamental mode}}(\omega) + P_{\text{scattering}}(\omega) + P_{\text{metal loss}}(\omega) \tag{4}
\]

where \(P_{\text{total}}(\omega)\) is the total optical power leaving the dipole source, \(P_{\text{metal loss}}(\omega)\) is the power lost to metal, and \(P_{\text{fundamental mode}}(\omega)\) is the power in the fundamental mode of the waveguide which was found by taking an overlap integral between the eigenmode solution and the simulated waveguide field profile. Note that the product of these efficiencies gives the fraction of the total optical power coupled to the fundamental waveguide mode. Additionally, we calculated the average antenna efficiency and waveguide coupling efficiency. Below are the explicit definitions for \(\eta_{\text{antenna}}\) and \(\eta_{\text{WC}}\):

\[
\eta_{\text{antenna}} = 0.96 \times \frac{\int \eta_{\text{antenna}}(\omega)F(\omega)L(\omega)d\omega}{\int F(\omega)L(\omega)d\omega} \tag{5}
\]

\[
\eta_{\text{WC}} = \int \eta_{\text{WC}}(\omega)\eta_{\text{antenna}}(\omega)F(\omega)L(\omega)d\omega \tag{6}
\]

where 0.96 is the spatial average for the antenna efficiency. Note that the polarization dependence was negligible for both average efficiencies, since a dipole oriented along the width of the LED
sees much greater enhancement than a dipole oriented along the length. Additionally, the spatial dependence was negligible for the waveguide coupling efficiency.

These average values could now be used to calculate relevant device metrics since they represent the average response of a carrier in the device. Two important metrics are the power in the fundamental mode of the waveguide and the 3dB frequency, given in Eqs. (7) and (8), respectively.

\[ P_{\text{fundamental mode}} = F_{\text{avg}} \eta_{\text{antenna}} \eta_{\text{WC}} \hbar \omega B_0 N^2 V \]  
\[ f_{\text{3dB}} = \frac{2F_{\text{avg}} B_0 N}{2\pi} \]  

where \( B_0 \) is the radiative recombination coefficient, \( N \) is the carrier concentration, \( V \) is the active region volume, and \( f_{\text{3dB}} \) is the 3dB modulation frequency assuming the radiative recombination rate is dominant. If we assume \( F_{\text{avg}} = 164, B_0 = 10^{-10}\, \text{cm}^3\, \text{s}^{-1} \) [26], and \( N = 2 \times 10^{19}\, \text{cm}^{-3} \) we could reach a 3dB frequency of 104GHz.

**Inverse design**

In this work we used the Berkeley Photonic Inverse Design package, originally described in [19]. The inverse design optimization problem that was solved can be written as the following:

\[ \max_{\theta} \sum_{\omega} c_{\omega} T_{\omega}(x, r) : \text{Radius of Curvature} \geq 100\, \text{nm} \]  

where \( \theta \) denotes the optimization parameter space – which in this case is the interface between InP and Ag in the metal-optic waveguide coupler region, \( \omega \) is an index that defines the frequency bandwidth of the optimization, \( T \) is the Poynting vector evaluated at positions \( r \) in the waveguide for electric and magnetic fields abbreviated by vector \( x \), and \( c \) is a user-defined weight chosen for each frequency index. Finally, we included an optimization constraint on the radius of curvature to ensure fabricability. A brief discussion of the limitations of our inverse design implementation follows.

The objective function that was used in inverse design does not give individual control over our figures of merit, \( F_{\text{avg}}, \eta_{\text{antenna}}, \) and \( \eta_{\text{WC}} \). Consequently, we included the weights, \( c \), in the objective function to provide this control. An additional limitation comes in reference to Fig. 4(c) where the length of the metal along the coupler section sidewalls is not perturbed. Since it is undesirable to have metal along the sidewalls of the coupler section (XY plane) with a different length than the metal on top of the waveguide (XZ plane), the metal on top of the waveguide effectively constrained the designable region. Therefore, we used several metal lengths as initial conditions for inverse design optimization.

Lastly, one of the most important considerations for our choice of the waveguide coupler structure in Fig. 4 was its compatibility with top-down fabrication. In other words, since the entire ridge must share the same etch mask, it must also share the same 2D cross-sectional shape in the XY plane. Therefore, a geometrical constraint is required in the inverse design optimization to maintain the conformal nature of the ridge which is composed of several materials. Such a constraint was unavailable in our basic implementation of inverse design. We imposed this constraint ad hoc by updating the SOG-Ag and SiO\(_2\)-Ag interfaces every three iterations to match the changing InP-Ag interface, but no significant convergence issues were encountered.

**Field profiles**

In Figs. 8(a)-8(c) we plotted the \( E_x \) and \( E_y \) field profiles of the mode in the InP waveguide at 1550nm for the structures given in Figs. 2(a)-2(c), respectively. In each structure the electric field profiles have been self-normalized by the maximum electric field magnitude.
Fig. 8. $E_x$ and $E_y$ field profiles for (a) antenna-LED on single-mode InP waveguide and SiO$_2$ ridge, (b) antenna-LED on single-mode InP waveguide with metal wrapped around waveguide facet, and (c) antenna-LED on single-mode InP tapered waveguide with metal wrapped around waveguide facet and sidewalls.
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