

Robust optimization of adiabatic tapers for coupling to slow-light photonic-crystal waveguides

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Abstract: We investigate the design of taper structures for coupling to slow-light modes of various photonic-crystal waveguides while taking into account parameter uncertainties inherent in practical fabrication. Our short-length (11 periods) robust tapers designed for $\lambda = 1.55 \mu\text{m}$ and a slow-light group velocity of $c/34$ have a total loss of $< 20\text{dB}$ even in the presence of nanometer-scale surface roughness, which outperform the corresponding non-robust designs by an order of magnitude. We discover *a posteriori* that the robust designs have smooth profiles that can be parameterized by a few-term (intrinsically smooth) sine series which helps the optimization to further boost the performance slightly. We ground these numerical results in an analytical foundation by deriving the scaling relationships between taper length, taper smoothness, and group velocity with the help of an exact equivalence with Fourier analysis.

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OCIS codes: (050.1755) Computational electromagnetic methods; (130.0250) Optoelectronics; (130.5296) Photonic crystal waveguides; (250.5300) Photonic integrated circuits; (350.4238) Nanophotonics and photonic crystals.

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1. Introduction

In this paper, we combine large-scale optimization, an increasingly popular tool in nanophotonics [1–16], with robustness and slow light for the problem of coupling two dissimilar waveguides [17–36]: here, a conventional dielectric waveguide and a periodic waveguide with a "slow-light" band edge [37–39] where the group velocity approaches zero. We start with the basic idea of an "adiabatic taper," a gradual transition that allows wide-bandwidth efficient coupling [40], and apply optimization (~ 1000 parameters) to design the best "profile" of the taper rate for a given taper length L , in order to minimize the tradeoff between taper length L and taper reflectivity R . We obtain $< 20\text{dB}$ reflection for L of only a few periods, but we show that the problem becomes intrinsically more difficult as the group velocity decreases, and the resulting optimized designs become more and more counterintuitive. A key idea in our approach is the use of *robust* optimization [41–45]: optimization that takes into account manufacturing uncertainty (e.g. fabrication disorder or errors in the dielectric constant or operating frequency) by always optimizing the *worst-case* perturbation to any design. Building on our previous work [43], we show that traditional "nominal" optimization (i.e., assuming no uncertainty) in photonic devices such as this one can easily lead to disaster: an optimized device that performs well only because of some delicate interference cancellation, and whose performance advantage is destroyed even by tiny manufacturing errors. In contrast, the robust optimum degrades much more gracefully in the presence of errors: by taking into account the possibility of errors from the beginning, the robust optimization procedure tends to avoid designs that rely on delicate cancellations. Rather than expensive simulations of the full Maxwell equations performed during the optimization procedure [18,20,21,25,34–36], rapid semi-analytical coupled-mode theory (CMT) [40] calculations are possible for the taper-design problem [37,43]—these initially perform small Maxwell simulations only for the periodic building blocks of the taper to determine the waveguide modes, and subsequently compute a simple integral (equivalent to a weighted Fourier transform) to find the reflectivity of any given taper profile. CMT trades off efficiency for generality, but is an indispensable tool to make large-scale optimization feasible for gradual tapers, especially in 3d. We find that, in the CMT context, the robustness helps us in another way: by comparison to brute-force scattering-matrix calculations [46], we find that our designs are also robust to computational approximations. Even with robustness, however, as the group velocity becomes lower we show that large-scale (many-parameter) optimization tends to push towards an artificial solution that exaggerates discrepancies between the optimization model and the physical circumstances (e.g. modelling errors and/or imperfect uncertainty models), a tendency that can be combatted by building in *a posteriori* observations about the nature of the robust optima. In particular, we observe that the robust optima tend to be smooth, slowly-oscillating shapes that can be parameterized as a linear taper plus a truncated sine series with a few terms, and by using this information *a priori*, in *addition* to robust optimization, we obtain

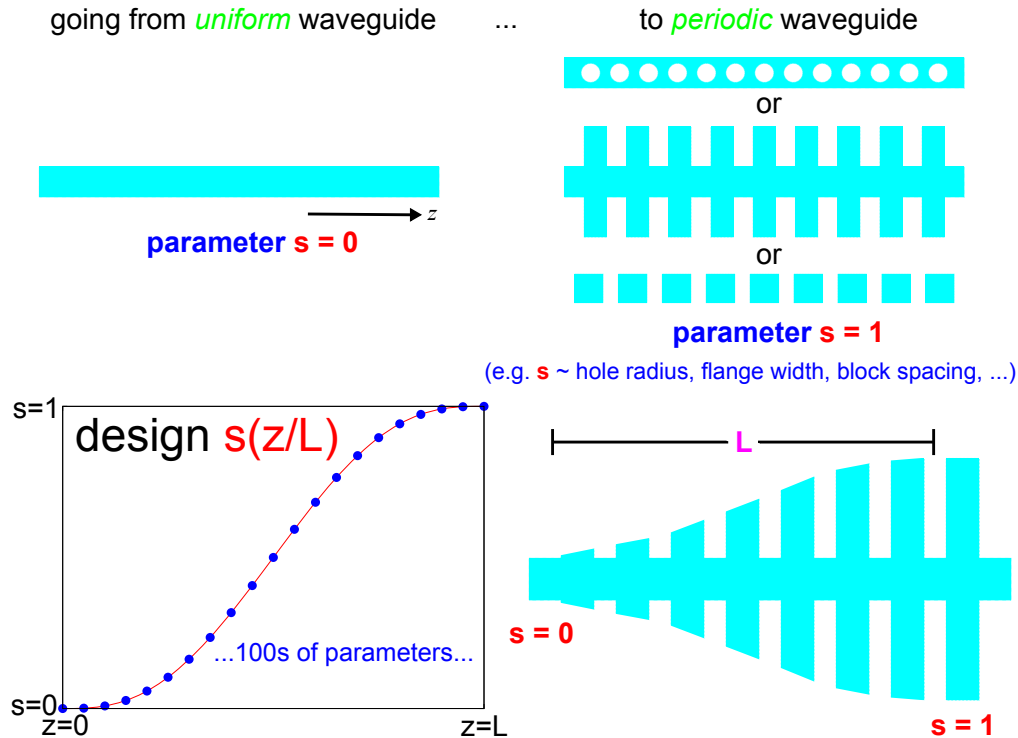


Fig. 1. Schematic taper design problem, with a transition between two waveguides characterized by a dimensionless parameter $s \in [0, 1]$. The taper goes from a uniform dielectric waveguide ($s = 0$) to a periodic waveguide ($s = 1$), with $0 < s < 1$ describing intermediate structures (e.g. $s \sim$ hole radius, flange width, or block spacing in the structures shown at right). A taper design (bottom) is a “shape” function $s(z/L)$ (for $z \in [0, L]$) describing a continuous transition from $s(0) = 0$ to $s(1) = 1$. For optimization, we parameterize s by its values at uniformly spaced points and linearly interpolate in between (bottom left).

an improved design at very low group velocities. Although we show analytically that smoothness reduces taper reflections *asymptotically* for long tapers, the desirability of smoothness for optimized short tapers is not as apparent, especially in light of many previous coupler designs employing abrupt transitions [20, 23, 25, 26, 30, 33, 34, 47, 48].

The coupling of optical modes from one structure to another is crucial for enabling complex integrated photonic devices. A particular challenge is posed by slow-light waveguides, which are useful since their low group velocity enhances many types of light-matter interaction [39] as well as enhancing dispersion effects [37]. For example, the slow-light increase of the field intensity boosts the optical force in optomechanical systems [49–51], and it also enhances nonlinear effects for a variety of applications [39, 52–54]. Many designs have been proposed for coupling dissimilar waveguides (in most cases at moderate group velocities), including designs based on butt-coupling [23, 26], mode-field matching [20, 25, 30, 47], anti-reflection coatings [33, 34], resonant transmission [48], and gradual taper transitions [17–19, 21, 22, 24, 27–29, 31, 32, 36, 37, 40, 43]. Most of these works involved only a small number of tunable degrees of freedom, which (combined with the moderate group velocities) helped to avoid the ultra-sensitive nonmanufacturable designs that tend to arise when many degrees of freedom are included; hence, they were able to disregard uncertainties during

the design process. Resonance can be used to couple to slow light, but is intrinsically narrow-band and relies on a delicate cancellation represented by a forced impedance matching (although, being a single parameter, manufacturing errors could conceivably be compensated by post-fabrication tuning) [48]. Strong frequency and parameter sensitivity was also encountered in the optimization of a coupler over many degrees of freedom [7]. To address a similar problem in our earlier work, we introduced one simple way of incorporating robustness by optimizing the worst-case performance over a large ($\pm 30\%$) range of rescaled taper lengths for the same shape [37]. In particular, we designed an adiabatic taper for coupling to a slow-light 3d flanged waveguide (with a moderately low group velocity of $c/10$) having low reflection (< 20 dB), and optimizing over shapes parameterized by a few parameters (degree-4 polynomials) [37]. However, it is desirable to develop a framework in which more general uncertainties can be incorporated. To this end, we recently demonstrated a method for designing waveguide tapers that takes into account uncertainties in the operating frequency and taper shape while using a large number (hundreds) of free parameters [43]. As a proof of concept, we designed a fixed-length (30 periods) taper (to periodic 2d blocks) by smoothly varying the air gaps, coupling to a mode at a moderate group velocity of $c/4$ [43]. Here, we extend that work to a more realistic waveguide taper (a waveguide with periodic side flanges, which can be gradually extended while avoiding arbitrarily narrow air gaps), closely analogous to the fabricatable [55–57] 3d flanged waveguide considered in Ref. 37, but in two dimensions so as to be amenable to brute-force validation of its performance in the face of fabrication imperfections (surface roughness). Furthermore, rather than looking at a fixed taper length as in our previous works, we investigate the central engineering tradeoff in this problem: the tradeoff between performance and taper length, by comparing separately-optimized structures at different lengths. We go down to a group velocity of $c/34$, where the taper problem becomes even more challenging (both physically and in the optimization sense, e.g. we find that low group velocity required more algorithmic effort to avoid being trapped in poorly-performing local optima, and also requires more care to maintain the validity of CMT). Finally, we extend the asymptotic analysis of the adiabatic limit (taper length $\rightarrow \infty$) from our previous works [37, 40] to address the interplay between taper smoothness, group velocity, and reflection (with the help of an exact equivalence to Fourier analysis that we derive here).

In a sense, all engineering design is a problem of optimization: choosing some design parameters \mathbf{p} to optimize some objective $O(\mathbf{p})$, possibly subject to some constraints. Large-scale optimization (sometimes called “inverse design”) is simply optimization in the regime where there are many parameters, so many that one cannot easily intuit the form of the solution. (With many parameters, it is crucial that one evaluate the gradient $\nabla_{\mathbf{p}}O$ analytically, which can be efficiently achieved by an adjoint method [58].) There are many algorithms to solve optimization problems of many different kinds, but robust optimization is not about the choice of algorithm, it is about changing the optimization *problem*. Instead of solving a *nominal* optimization like $\min_{\mathbf{p}} O(\mathbf{p})$, in which the optimization process assumes that O is known exactly with no uncertainties, robust optimization techniques transform the problem to incorporate uncertainties. If the uncertainties are described as unknown values \mathbf{v} in some set \mathcal{V} (e.g. the error bars of manufacturing variability), then one way to “robustify” the problem is to optimize the *worst* case, $\min_{\mathbf{p}} [\max_{\mathbf{v}} O(\mathbf{p}, \mathbf{v})]$. (There are also other possibilities, such as optimizing the average case, but worst-case optimization benefits from the availability of many practical algorithms [43]. Reference 45 employed a simplified worst-case analysis for a waveguide-design problem, in which the worst of three designs was optimized.) Most previous work on robust optimization focused on “convex” optimization problems [59]—essentially, problems with no suboptimal local minima, which can therefore be efficiently solved exactly. However, design problems in optics, including the taper design problem here, are typically nonconvex: one cannot in general find

the global optimum (except in the case of small parameter spaces that can be searched exhaustively [60, 61]) and must settle for an approximation (a local optimum). Reference 43 developed an effective technique to approximately solve non-convex *robust* optimization problems, combining approximate pessimization (worst-case analysis) with multi-scenario optimization. (A somewhat more complicated algorithm, which combined pessimization by gradient ascent from multiple sample points in \mathcal{V} with optimization by gradient descent along a direction determined by solving a second-order cone problem, was applied to a microwave scattering problem by Ref. 44.) Reference 43 also showed the effectiveness of a successive-refinement strategy (gradually increasing the number of degrees of freedom) to avoid being trapped in poor local optima. (In fact, we now find that the robustness itself helps to avoid being trapped in poor local optima, so much so that it was helpful to artificially enlarge the uncertainty set \mathcal{V} .)

To set the stage for our remaining paper, we begin by more precisely defining a taper-design robust-optimization problem (as in Ref. 43), depicted schematically in Fig. 1. We are coupling a uniform dielectric waveguide to a periodic (period a) waveguide, e.g. a dielectric waveguide pierced by a sequence of holes [38, 62, 63] or with periodic side flanges [55–57]. A continuous transition from the uniform waveguide ($s = 0$) to the periodic waveguide ($s = 1$) is described by a dimensionless parameter $s \in [0, 1]$; for example, s could be proportional to the hole radius (if we taper by gradually increasing the hole radii) or to the flange width (if we gradually taper the flanges outwards). A *taper design* is then described by a continuous profile $s(z/L)$, which characterizes all intermediate structures for $z \in [0, L]$. [This easily generalizes to the case of multiple taper parameters $s_n(z/L)$ that are varied independently, e.g. hole radius and waveguide width or flange width and height, but we found that a single taper parameter sufficed to obtain good performance.] As we review below (and have argued elsewhere [37, 40, 43]), the taper losses are usually dominated by reflections (as opposed to radiative scattering), especially for slow light, so it is sufficient for us to minimize the reflectivity $R[s(z/L), \mathbf{v}, L]$, which is a functional of both the taper shape $s(z/L)$ and a vector \mathbf{v} of small *uncertainties* (in some set \mathcal{V}), for a given design length L . For example, the uncertainties \mathbf{v} could include (as components) some uncertainty $\Delta\omega$ in the operating frequency, imperfections $\Delta s(z/L)$ in the shape, and/or uncertainty ΔL in the taper length. As described above, the robust design problem is then to minimize the worst-case reflection, a “minimax” problem:

$$R_{\min}(L) = \min_{s \in \mathcal{S}} \max_{\mathbf{v} \in \mathcal{V}} R[s, \mathbf{v}, L], \quad (1)$$

where \mathcal{S} is some set of allowed taper shapes. To begin with we parameterize $s(z/L)$ by its values $s(n/N) \in [0, 1]$ at N equally spaced points n , with $s(0) = 0$ and $s(1) = 1$, and then linearly interpolate s between these points as shown in Fig. 1. (This can be thought of as a “tent function” basis [58].) We also constrain the slope $|s'(z/L)| < 5$ —without some constraint on the smoothness of s , the optimization strays too far outside the bounds of validity of CMT and numerical difficulties arise. At the end of the paper, we also consider an alternative parameterization $s(z) = z/L + (\text{sine series})$, with a linear constraint to enforce $s \in [0, 1]$. By the adiabatic theorem [40], $\lim_{L \rightarrow \infty} R[s(z/L), 0, L] = 0$ (in the absence of surface roughness or other uncertainties that cause scattering), but the goal of optimization is to determine the best tradeoff curve $R_{\min}(L)$ (with a *different* optimal shape s for each L).

2. Analytical and computational methods

There are two computational challenges: first, solving Maxwell’s equations to obtain R for any given s , \mathbf{v} , and L ; and second, solving the optimization problem (1) for R_{\min} . These two questions are related because a very efficient method to compute R is desirable in order to rapidly explore a large parameter space (s, \mathbf{v}, L) during optimization. To address this challenge,

we first review CMT and its application as a numerical method, and also discuss its analytical implications for the asymptotic properties of gradual tapers. We also compare CMT with more “brute-force” simulation algorithms, which are used both for validation of CMT and for post-optimization evaluation of our designs in the face of disorder. Finally, we briefly review the optimization algorithm, which was developed in detail in our previous work [43].

2.1. Coupled-mode theory and the adiabatic limit

In order to compute R , as in our previous work [37, 43] we employ the coupled-mode theory (CMT) developed in Ref. 40. The basic idea is to expand the field in the waveguide in the basis of the Bloch eigenmodes of periodic waveguides—here, the waveguide modes corresponding to the intermediate structure $s(z/L)$ is used to expand the fields at that z . Abstractly, if the electromagnetic field is $\psi(z)$ (with xy coordinates omitted), we write $\psi(z) = \sum_n c_n(z) \psi_n(z) \exp[i \int^z \beta_n(z') dz']$, where the $\psi_n(z)$ are the Bloch eigenmodes at z , β_n is the corresponding propagation constant (or wavevector), and c_n is the expansion coefficient. When this expansion is substituted into the Maxwell equations, a set of coupled ODEs for $c_n(z)$ is obtained (the “coupled-mode” or “coupled-wave” equations) [40]. In the $L \rightarrow \infty$ limit, the adiabatic theorem states that the expansion coefficients are constants [$c_n(z) \rightarrow c_n(0)$], while for a finite L we can apply a slowly varying envelope approximation (SVEA) to compute the corrections to this limit. In the SVEA, assuming we start with a single incident mode $c_n(0) = \delta_{n0}$, to lowest order in the rate of change one finds that the reflected-wave amplitude c_r is [40]:

$$c_r = \int_0^1 du s'(u) \sum_k \frac{M_k[s(u)]}{\Delta\beta_k[s(u)]} e^{iL \int_0^u \Delta\beta_k[s(u')] du'} . \quad (2)$$

Here, $M_k(s)$ is a coupling matrix element (an overlap integral $\langle \psi_i | \dots | \psi_r \rangle$) of the incident and reflected fields with the geometric variation, and $\Delta\beta_k(s) = \beta_r(s) - \beta_i(s) + 2\pi k/a(s)$ is a phase-mismatch factor between the incident (i) and reflected (r) modes summed over all Brillouin zones (all integers k). In this paper, the M_k and $\Delta\beta_k$ parameters were obtained from a planewave-expansion method [64]. In practice, the sum over k converges rapidly [40] so we only included $|k| < 3$. The reflected power is then $R = |c_r|^2$. Computation of the gradient $\nabla_s c_r$ is described in Ref. 43. (It is important to contrast this Bloch-mode expansion with older coupled-wave approaches that expand in the basis of *uniform* waveguide modes of each cross-section, which is ineffective as a semi-analytical technique for strongly periodic structures in which the cross section is rapidly varying [40]. A Bloch-mode basis, on the other hand, experiences no scattering at all from the periodicity itself—it only undergoes intermodal scattering when the periodicity is broken by the taper, and is therefore a rapidly converging basis for gradual taper transitions of periodic structures, including structures whose unit cells contain discontinuities such as air gaps [40].)

In principle, the total loss ($1 - \text{transmission}$) includes radiative scattering in addition to reflection (assuming single-mode waveguides so that there is no other inter-modal reflection). However, the reflected power tends to dominate [40], especially for slow-light modes (low group velocity $v_g = d\omega/d\beta$), as can be argued from (2) [37]. First, at a quadratic band edge in a periodic waveguide, $\Delta\beta \sim v_g$ (for the k term corresponding to modes $\beta = \pi/a \pm \Delta$ coupled in adjacent Brillouin zones)—this both decreases the denominator in (2) and decreases the phase mismatch. Second, the modes in coupled-mode theory are normalized to unit power [40], and hence the fields scale $\sim 1/\sqrt{v_g}$ and there is an additional $1/v_g$ factor in M for coupling slow-light incident and reflected modes, versus only a $1/\sqrt{v_g}$ factor in M for coupling slow-light incident to non-slow scattered waves [37].

In order to understand the validity of CMT and the precise scaling with group velocity, we must have a better understanding of the adiabatic limit. A particularly elegant approach

is to make a change of variables to transform (2) into a Fourier integral, at which point all of the well-known properties of Fourier transforms can be invoked. Omit the k summation for simplicity (e.g. focus on the dominant k term). The key point is that one generally (with rare exceptions [65]) considers adiabatic transitions in which the incident and scattered modes are never degenerate in β , so that $\Delta\beta$ is always nonzero. This is certainly true for the case of reflections. The function $x(u) = \int_0^u \Delta\beta_k[s(u')]du'$ is therefore monotonic, and one can invert it to $u(x)$ and change variables $u \leftrightarrow x$. We obtain precisely a Fourier integral:

$$c_r = \int_{-\infty}^{\infty} dx s'(u(x)) \frac{M_k[s(u(x))]}{\Delta\beta_k[s(u(x))]^2} e^{iLx}, \quad (3)$$

where we are free to extend the integration range since $s' = 0$ outside the taper. As long as s is continuous, so that s' contains no delta functions, this $\rightarrow 0$ for $L \rightarrow \infty$ because L is simply the “frequency” of a convergent Fourier transform. Furthermore, the *rate* at which $c_r \rightarrow 0$ with L is well known in Fourier theory to depend on the *smoothness* of the integrand [66, 67], which in this case is determined by the smoothness of s' (including the taper endpoints). For example, if s is a simple linear taper with discontinuous slope s' at the taper ends, then the Fourier transform (due to the discontinuity) scales as $c_r \sim 1/L$, hence the reflections go as $1/L^2$ asymptotically [37, 40]. More generally, if s has endpoint discontinuities in its ℓ -th derivative and is otherwise smooth, then $|c_r|^2 \sim 1/L^{2\ell}$ [66, 67] (we previously analyzed a related point in the context of PML absorbing boundaries, where the Fourier analogy was not so exact [68]). Similarly, the group-velocity scaling depends on the smoothness of s . For the case of a linear taper, or any taper with discontinuous s' , the reflection goes as $|c_r|^2 \sim |M/\Delta\beta|^2/L^2 \sim 1/(Lv_g^3)^2$, or equivalently we must have $L \sim 1/v_g^3$ to obtain a fixed reflection [37, 69]. For smoother tapers, the convergence analysis of the Fourier integral involves integration by parts to apply additional derivatives to s until the discontinuity is reached [66–68], which gives additional $du/dx = 1/\Delta\beta$ factors by the chain rule. Hence, the generalization to a discontinuity in the ℓ -th derivative is a scaling $|c_r|^2 \sim |M/\Delta\beta|^2/(L\Delta\beta)^{2\ell} \sim (1/v_g^4)/(Lv_g)^{2\ell}$, or $L \sim 1/v_g^{1+2/\ell}$. The consequence of this scaling is that a tradeoff of taper length with group velocity becomes (asymptotically) better for *smoother* tapers, approaching $L \sim 1/v_g$, and so smoothness—eliminating high-frequency Fourier components—of the taper shape may be especially important for slow light. On the other hand, the optimum taper shape is very different for any given finite L than it is in the asymptotic limit—the rule is not simply “smoother is better,” because smoother tapers also tend to require a larger L to attain the asymptotic $1/L^{2\ell}$ behavior [68]. Optimization is required to determine the best shape for any finite L , especially for short L far from the asymptotic regime.

2.2. Brute-force numerics and validation

CMT, when evaluated to lowest-order as in (2), is asymptotically exact in the limit of gradual tapers, but is only an approximation for the rapid taper transitions that are the goal of optimization because we are neglecting multiple-scattering effects. (Note that our expansion basis is that of *Bloch* modes [40], so multiple-scattering effects of the periodicity itself are treated exactly; it is only multiple scattering *between* Bloch modes due to the taper transition that are neglected.) Fortunately, the optimization will also tend to drive the taper shape precisely into the small- $|c_r|$ regime where CMT is accurate. However, to check the performance of our taper designs, we supplement the CMT with a brute-force numerical calculation based on an eigenmode-expansion scattering-matrix method (also called RCWA, the rigorous coupled-wave approximation) via the free CAMFR package [70]. CAMFR is also used as a final check of the robustness of the designs to fabrication errors, since in that method we can incorporate random

surface roughness in the taper (which requires a different coupled-mode theory technique to describe it accurately [71]). In general, we found that the robust-optimization approach produced designs that were robust even in the face of errors in the computational method, whereas we show below that nominal optimization produces designs whose performance is destroyed even by slight changes in the simulation accuracy.

Figure 2(a) shows a linear (forward and backward, double) taper between a uniform waveguide and a sequence of dielectric blocks ($\epsilon = 12$), for relatively “fast” light ($v_g \approx c/4$) in the TM (out-of-plane \mathbf{E}) polarization, with excellent agreement between CAMFR and CMT except for very short tapers with reflections $> 10\%$. This structure is convenient for validation [40, 43] because its piecewise-constant cross-sections are particularly efficient in CAMFR and allow us to study very long and gradual tapers, but it is relatively difficult to realize experimentally because its tapers involve many extremely narrow air gaps (that must be abruptly merged in practice once the limits of lithographic resolution are reached [72]). In Fig. 2(b), we instead consider a (TE-polarized) case of a waveguide with lateral flanges [55–57] operating close to the band edge where the group velocity is $\approx c/34$. This sort of geometry is experimentally attractive because a gradual taper involves no arbitrarily narrow features, and the TE polarization translates into a TE-like polarization in three dimensions that can be confined by much thinner structures than TM-like polarizations [38]. In this case, however the CMT only begins to converge to the CAMFR results (which we also check against a third numerical method, FDTD [73, 74]) for very long tapers, but this is not unexpected. Because of the slow light used here, the reflections are very large ($\sim 40\%$), and the first-order approximation in our CMT is expected to be inaccurate. For slow light, as explained above, a simple linear taper is a poor choice even if the taper can be made quite long: although CMT predicts an asymptotic $1/L^2$ scaling of the reflection, we would need to go to much larger lengths to observe this scaling for slow light. [Unfortunately, CAMFR is far more expensive for the taper in (b) than for the taper in (a), due to the nonconstant cross-sections in the former, while FDTD is also too expensive to simulate a very gradual taper.] As we show below, however, optimizing the CMT in the slow-light case nevertheless yields a (much more counterintuitive) design that performs well even in the brute-force CAMFR check.

2.3. Robust-optimization algorithm

The basic optimization algorithm, as described in Ref. 43, is sequential linear programming (SLP) with a trust-region constraint [75, 76]. In order to implement the robustness [the inner $\max_{\mathbf{v}}$ of (1)], the method uses the gradient $\nabla_{\mathbf{v}}R$ to estimate the worst-case \mathbf{v} parameters for the current shape s (and in fact accumulates a memory of ten such worst cases over the course of the optimization that it uses for subsequent steps), and thus transforms the continuous $\max_{\mathbf{v}}$ into a discrete “multi-scenario” maximization over a finite set of worst-case candidates [43].

Reference 43 also introduced a technique of “successive refinement”: we gradually increase the number of degrees of freedom (from 1 to 1024, roughly doubling in each step), using the optimized coarser structures as starting points for optimization of the finer structures. This procedure has two benefits: it both increases the robustness of the design (by making it more robust to coarsening the discretization of s) and also tends to avoid becoming immediately trapped in local minima (although we cannot guarantee that the final result is a global minimum).

We found that the precise details of the set \mathcal{V} of uncertainties makes relatively little difference—putting in *any* robustness tends to force the optimization to avoid delicate cancellations that would be sensitive to any errors. However, some care is required in the case of slow light because of the presence of a band edge beyond which the guided mode no longer exists. As the band edge is approached, any uncertainty $\Delta\omega$ in the operating frequency must be reduced to avoid going past this band edge. In practice, if a fabrication error were to shift

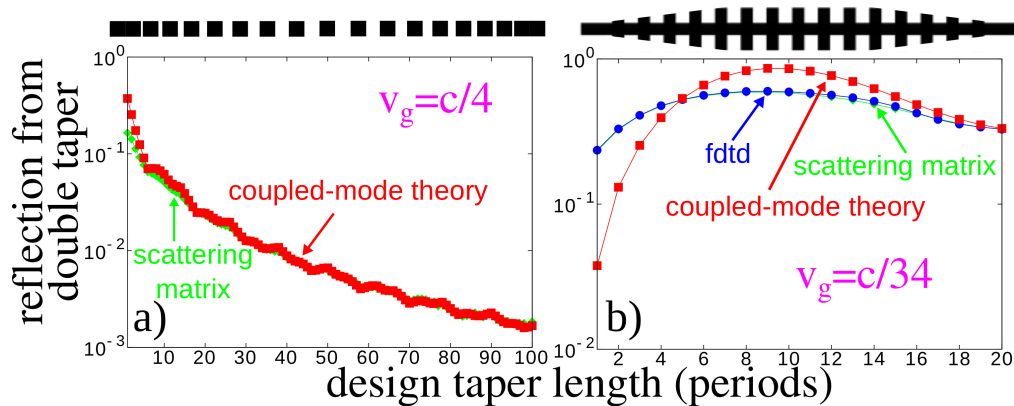


Fig. 2. Comparison of coupled-mode theory (CMT) calculation of reflection coefficient from double taper (from uniform to periodic to uniform) structure, using a simple linear profile $s(u) = u$, with two other brute-force numerical methods, scattering matrix (CAMFR [46]) and finite-difference time-domain (FDTD [74]). (a) 2d period a $0.4a \times 0.4a$ blocks example (top left) with TM operating mode at $v_g = c/4$ [40,43]. CMT and CAMFR agree well. (b) 2d period- a flanged waveguide (inner width a , outer width $2a$, 50% duty cycle) with TE operating mode at $v_g = c/34$, adapted from Ref. 37 (top right). For such slow light, the scattering from a short linear taper is too large for CMT to be valid, but optimization of the taper shape will drive the reflections low enough for the CMT calculation to be suitable.

the band edge slightly, an application requiring slow light would have to either adjust the operating frequency accordingly or perform post-fabrication tuning (e.g. by thermally changing the refractive index) in order to keep v_g fixed. Therefore, to reflect this situation of fixed v_g , we did not include any uncertainty in ω . However, in order to represent the possibility of error in the phase velocity (ω/β) that could result from such post-fabrication tuning, we instead included an uncertainty ΔL in the taper length L [equivalent to an overall shift in β by (2)]. Since $\partial\beta/\partial\omega$ diverges as $v_g \rightarrow 0$, we increased the uncertainty in L (and hence in β) as we decreased v_g —failing to do this resulted in designs that were overly sensitive to fabrication errors in our simulations. Furthermore, we found that decreasing v_g made the optimization increasingly susceptible to being trapped in poor local minima—intuitively, the increased reflections in the slow-light regime also increase the number of opportunities for delicate cancellations—and increasing ΔL helped to combat this tendency. We also included random perturbations in s (at each discretized s point), but we found that this made little difference in the resulting design once ΔL was sufficiently large.

3. Results

We now discuss the results of optimizing and simulating taper designs for the two different waveguides of Fig. 2, considering both slow light and moderate group velocities, for both nominal ($\min_s R$) and robust ($\min_s \max_v R$ optimization), with and without introducing “fabrication disorder” (surface roughness) in the simulation (after optimizing).

3.1. Periodic blocks

To begin with, we return to the periodic (period a) sequence of $0.4a \times 0.4a$ blocks (dielectric constant $\epsilon = 12$ in air) from Fig. 2(a) that we studied in Ref. 43, operating at the same moderate

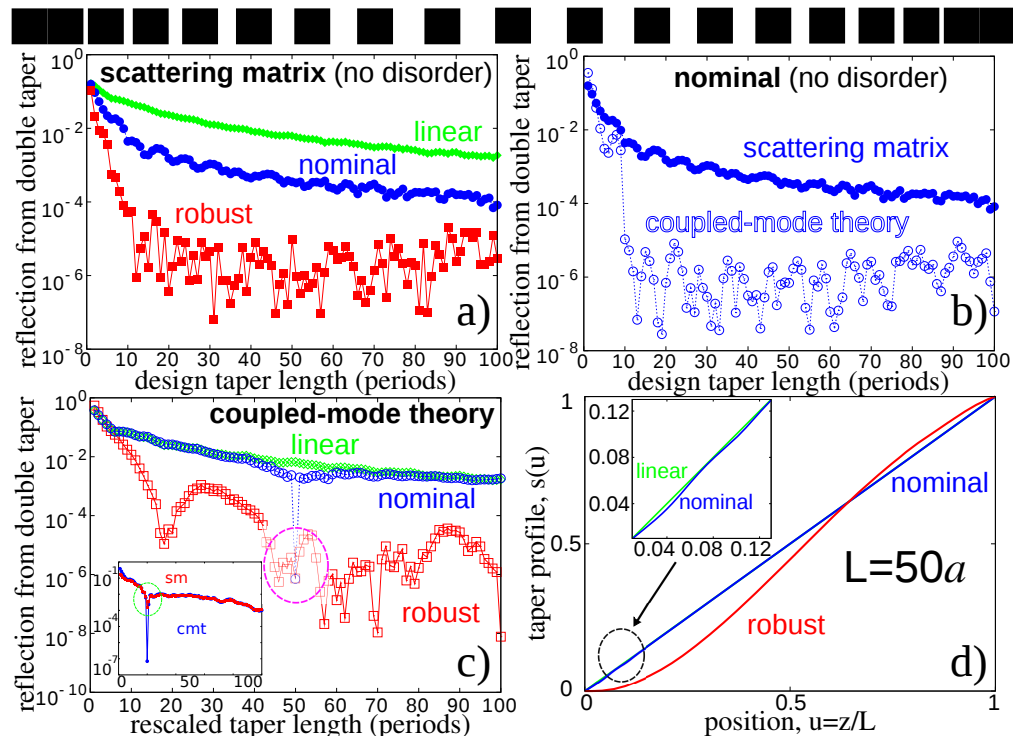


Fig. 3. Optimization results for taper structure of square blocks (operating TM mode with $v_g = c/4$) from Fig. 2(a), with block spacing as the taper variable (top: linear tapers). (a) Performance of three tapers (linear in green, nominal optimum in blue, and robust optimum in red, with the optimizations performed independently at each length L) computed using a brute-force scattering-matrix method (CAMFR [46]) (with no disorder introduced). (b) Performance of nominal taper (optimized independently at each taper length) computed using two different methods (CMT and CAMFR)—the large disparity is due to the nominal optimum relying on a delicate interference cancellation that is destroyed even by the slight numerical differences between the two techniques. (c) Performance of linear, nominal, and robust tapers designed at $L = 50a$ and then rescaled to other taper lengths: the nominal optimum relies on a delicate cancellation that only works close to $L = 50a$. Inset compares CMT and CAMFR for the $L = 20a$ design rescaled to different lengths, and illustrates that the two approaches agree everywhere except at $L = 20a$, where there is a delicate interference cancellation that is inherently irreproducible (non-robust), and at small L where the reflection exceeds 10% (causing CMT to break down). (d) Nominal and robust taper profiles $s(u)$ designed at $L = 50a$: the nominal design is only slightly different from a linear taper, with the slight changes (inset) sufficient to create a delicate reflection cancellation.

group velocity of $c/4$ and coupled to a uniform waveguide of width $0.4a$, which is a convenient test problem because of the ease of comparison with brute-force CAMFR simulation. Unlike our previous work, however, we now perform the optimization of s separately for every taper length $L \in [1, 100]a$, in order to examine the tradeoff of optimal R_{\min} with L . We then simulate each of the resulting taper designs in CAMFR in order to verify their performance.

The results are shown in Fig. 3(a), and exhibit a surprising phenomenon: even when *no disorder* (no roughness) is introduced into the scattering-matrix (CAMFR) calculation, so that in principle it should be modeling exactly the same system as the CMT calculations used during optimization, the nominal optimum exhibits *worse* performance than the robust optimum (and both are better than a simple linear taper). Mathematically, one would expect that the nominal optimum should always perform at least as well as the robust optimum when the disorder is set to zero, simply because $\max_{\mathbf{v}} R[s, \mathbf{v}] \geq R[s, 0]$. The reason for the behavior in Fig. 3(a) is simple, however: the nominal optimum relies on such a delicate cancellation effect that even the slight difference in simulation accuracy between CAMFR and CMT (both will have simulation errors, but the errors will be different) is sufficient to radically degrade the performance of the nominal optimum, while the robust optimum still performs well. As shown below, when the nominal and robust optima are evaluated in CMT, the nominal performance is indeed slightly better.

This discretization-error degradation in the nominal optimum can be seen in Fig. 3(b), which compares the CMT and CAMFR calculations for the nominal optimum at each L . For very short tapers, they make comparable predictions, but once the taper is about $10a$ in length the optimization is able to engineer a delicate cancellation that causes the CMT reflections to suddenly drop by four orders of magnitude (at which point they become limited by numerical errors and cease to improve further). Even the slight difference in discretization error induced by the switch from CMT to CAMFR, however, is enough to destroy this cancellation. (In our previous work, we showed for this structure that the robust optimum remained an order of magnitude better than the nominal optimum even after additional disorder is intentionally introduced into the CAMFR calculation [43]; we consider such disorder in the next section.) The agreement of CMT and CAMFR everywhere *except* at the point of this delicate cancellation is demonstrated below, using the inset of Fig. 3(c).

Another viewpoint on this delicate cancellation is shown in Fig. 3(c), which considers the design s for $L = 50a$, but then plots the performance of the same taper shape $s(z/L)$ when it is rescaled to other lengths L . The nominal optimum performs well only at the design length of $L = 50a$, and its performance immediately degrades to little better than a linear taper shape ($s(u) = u$) as soon as it is rescaled to a different L —this is a signature of a delicate destructive cancellation in the reflected wave that the nominal optimization forced to occur at $L = 50a$. The inset compares CMT and CAMFR for a rescaled $L = 20a$ design, and shows that the two agree except at $L = 20a$ where the non-robust cancellation occurs, which is destroyed by slight differences in discretization error as discussed above. In contrast, the robust optimum still performs well even when s is rescaled to lengths L very different from the L where the shape was designed—the robust optimum *does not rely* on a delicate cancellation that is easily destroyed. (As expected, the nominal optimum at $L = 50a$ is indeed slightly better than the robust optimum at that L , when the two are evaluated in CMT with no disorder.) The corresponding taper shapes s are shown in Fig. 3(d): while the robust optimum is a relatively smooth transition that flattens at the ends (reducing the s' discontinuities of a linear taper as might be expected from the asymptotic analysis), the nominal optimum is nearly identical to a linear taper, only deviating by a slight amount (inset) that is apparently tuned to force a reflection cancellation at $L = 50a$.

Finally, we should comment on one other interesting feature of Fig. 3(a): for the robust optimum, the reflections appear to decrease *exponentially* with L until reaching a “noise floor” around 10^{-6} imposed by numerical accuracy limitations. An exponential tradeoff of reflection

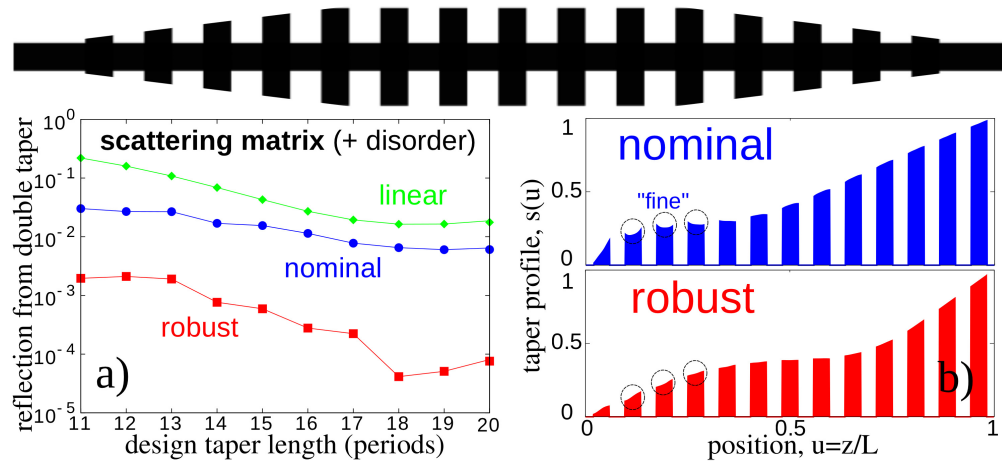


Fig. 4. Optimization results for taper from uniform to flanged waveguide (operating TE mode with $v_g = c/6$) from Fig. 2(b), with flange (outer) width as the taper variable (top: linear tapers). (a) Performance of three tapers (linear in green, nominal optimum in blue, and robust optimum in red, with the optimizations performed independently at each length L) computed using a brute-force scattering-matrix method (CAMFR [46]), where surface roughness ($\pm 10^{-3}a$ every $0.01a$) was introduced, averaged over 50 structures. The robust optimum maintains good (~ 30 dB) performance even in the presence of disorder, whereas the nominal optimum is greatly degraded. (b) Nominal and robust taper profiles designed at $L = 13a$ (vertical axis exaggerated for clarity): the nominal design includes fine cusps (circled) absent from the robust design, whose apparent function is to introduce reflection cancellations (which are spoiled by disorder).

with length is the ideal situation that would be attained asymptotically for an analytic taper shape (such as $s(u) = \tanh(u)/2 + 1/2$), due to the exponential convergence of the Fourier transforms of such analytic functions [67, 68], but this requires the taper to have an infinitely long “tail”, and in any case only applies asymptotically for large L . In contrast, optimization seems to attain a similar ideal tradeoff even for small L , even for finite-length tapers, albeit by changing the taper shape as a function of L . (Whereas the linear and nominal tapers show $1/L^2$ scaling.)

3.2. Periodic flanges

Next, we consider taper designs to couple to a waveguide with period- a dielectric ($\epsilon = 12$) flanges in air, as in Fig. 2(b): the flanges occupy 50% of each period, and extend to an outer diameter (flange width) of $2a$ from an inner diameter of a (matching the uniform waveguide). Again, we optimize separately at each L , in this case for $L \in [11, 20]a$ (shorter than in the previous section, both for computational tractability in brute force verification and also because short tapers are more practical).

To start with, in Fig. 4, we operate at a moderate group velocity $c/6$, at a frequency $\approx 1\%$ below the band edge of the fundamental mode. After optimization, we then simulated the resulting structures in CAMFR, but *modified* to include *disorder*: uniform random surface roughness with amplitude $\in [-10^{-3}, 10^{-3}]a$ (corresponding to \approx nm-scale surface roughness for operation at $\lambda = 1.55 \mu\text{m}$) added to each slice (“pixel”) of thickness $0.01a$ of the taper. Each result in Fig. 4(a) is the reflection averaged over 50 realizations of surface roughness. The robust optimum is more than an order of magnitude better in performance than the nominal optimum—

again, the nominal optimum is better in the CMT but relies on delicate cancellations that are destroyed by the surface roughness, although the nominal optimum is still slightly better than a simple linear taper. The robust design has reflections of ≈ 30 dB for a taper only $L = 11a$ in length. The reflection improves for longer lengths, but only slowly, and eventually starts to become worse—the reason is that there is a tradeoff introduced by the surface roughness, in that longer tapers are more gradual but also accumulate roughness-induced reflections over a longer length, and eventually the latter effect dominates. The nominal and robust designs for $L = 13a$ are shown in Fig. 4(b); note that the vertical axis is exaggerated for clarity. The robust $s(z/L)$ is a fairly smooth taper transition, exhibits some oscillatory behavior that seems hard to guess *a priori* (and s will become even more counter-intuitive when the group velocity is decreased below). The nominal optimum is even more strange, with some fine cusps appearing in the first few taper flanges that almost certainly *create* reflections, albeit in such a way as to exactly cancel other reflections (e.g. from the taper ends) in the absence of disorder.

Next, we move to a more challenging problem: coupling to the same structure, but at a frequency only 0.01% below the band edge of the fundamental mode, operating at a group velocity of $c/34$. In this case, a simple linear taper exhibits $> 30\%$ reflections for a taper length $L = 20a$. In Fig. 5(a), we show the CAMFR simulations of the optimized designs at each L , again modifying the structures to include surface roughness. The robust optimum here exhibits reflections < 20 dB, more than an order of magnitude better than the nominal optimum design, which is again only slightly better than a naive linear taper. The robust optimum, in fact, has a dip < 40 dB in its reflections at $L \in [13, 15]a$, apparently due to some destructive cancellation, but the dip disappears in Fig. 5(b) if we examine the total loss ($1 - \text{transmission}$) instead of just the reflections (which still dominate the loss for most L). Note that the losses again can be seen to *increase* with L , an effect of the increased scattering from roughness along a longer length. In order to obtain the good performance for the robust taper, we found that we needed to increase the amount of uncertainty ΔL in the optimization process to a relatively large value ($3a$), apparently to avoid being trapped in local minima. In fact, the nominal optimization seemed to immediately become trapped in a relatively poor solution, even for the CMT with no uncertainty—as shown in Fig. 5(c), the nominal optimum achieves > 20 dB reflections in the CMT, a performance that is destroyed when switching to CAMFR even with no surface roughness (due to discretization effects alone).

The nominal and robust optimum shapes $s(u)$ for $c/34$ are shown in the lower-left and top-middle panels of Fig. 6 (again with the vertical axis enlarged for clarity). The nominal optimum has even stronger cusps than in the $c/6$ velocity case, suggesting even more reliance on cancellations of strong interior reflections. However, even the robust optimum is highly oscillatory, with oscillations even within a single flange. Despite its good performance in the simulations of Fig. 5, this led us to wonder whether the oscillatory shape was somehow an artifact of the choice of parameterization of s . That is, is this merely a local minimum that we were trapped in as a consequence of discretizing s into piecewise linear (non-smooth) segments (tent functions) and gradually refining? To investigate this question, we repeated the robust optimization with an entirely different parameterization: $s(u) = u + (\text{sine series})$, where the sine series enforces the $s(0) = 0$ and $s(1) = 1$ boundary conditions. (The $0 \leq s \leq 1$ boundary conditions were imposed explicitly at 1000 points in u , which takes the form of a simple linear constraint added to the linear-programming steps.) Successive refinement was performed by repeatedly doubling the number of terms in the sine series (4, 16, 32, 64), setting the new terms to zero as the starting point for optimization. The resulting robust sine-series optima are shown in Fig. 6 (lower-right), and are clearly converging towards the same oscillatory robust optimum. The 64-term sine series $s(u)$ is superimposed on the original robust optimum in the top-middle panel, and can be seen to reproduce even many of the fine features within each flange.

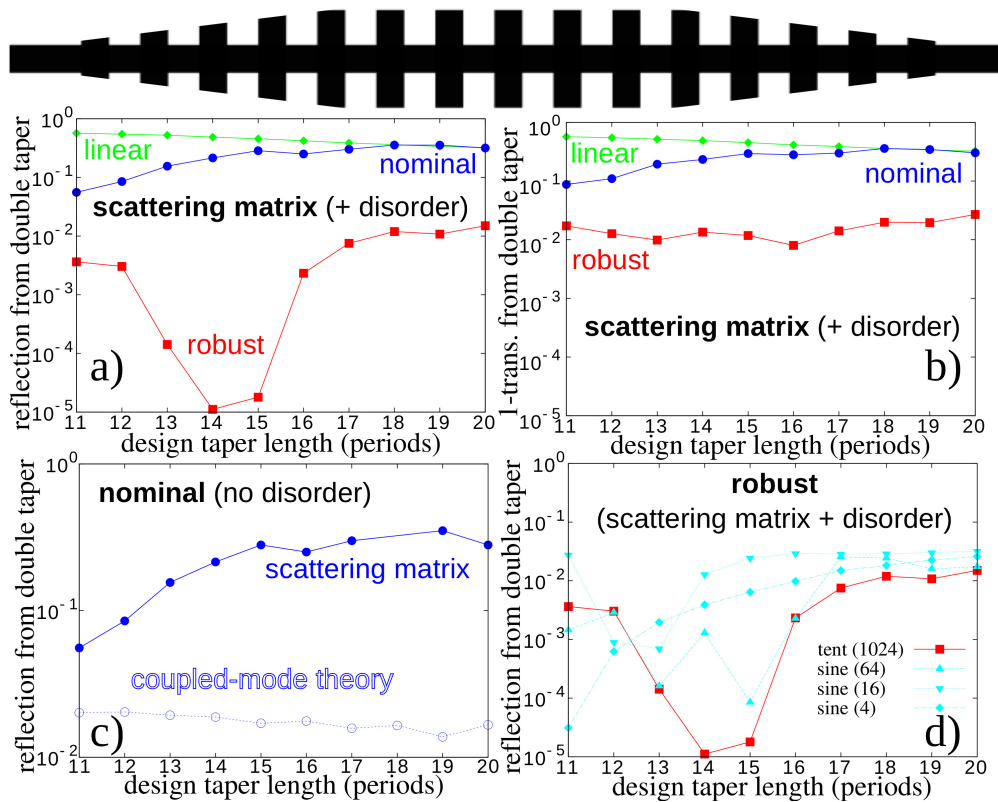


Fig. 5. Optimization results for taper from uniform to flanged *slow-light* waveguide (operating TE mode with $v_g = c/34$) with flange (outer) width as the taper variable (top: linear tapers). (a) Performance of three tapers (linear in green, nominal in blue, and robust in red, with the optimizations performed independently at each length) computed using a brute-force scattering-matrix method (CAMFR [46]), where surface roughness ($\pm 10^{-3}a$ every $0.01a$) was introduced, averaged over 50 structures. (b) Same as (a) but with $1 - \text{transmission}$: the inclusion of radiative scattering loss eliminates the optimization-created dip (cancellation) in the reflection losses from (a). As in Fig. 4, the robust optimum greatly outperforms the nominal optimum in the presence of disorder. (c) Even without disorder, the nominal optimum performs poorly in CAMFR compared to CMT: the slight differences in simulation accuracy are enough to spoil the nominal optimum. (d) Same as (a) but with robust optimization using the original (1024-point) piecewise-linear (“tent function”) parameterization (red squares) compared to robust optimization using a sine-series parameterization (cyan) with 4, 16, and 64 terms: the latter is converging towards similar performance as the former, and towards similar structures as seen in Fig. 6, so the robust optimum is not merely a local minimum obtained as a byproduct of the discretization choice.

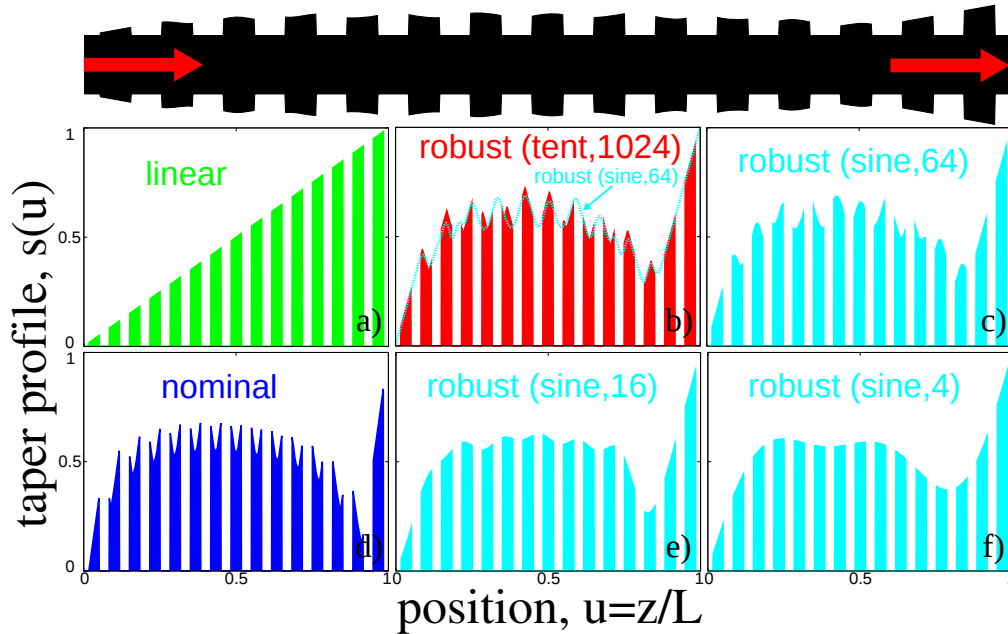


Fig. 6. Linear, nominal, and robust-optimum taper profiles from the slow-light ($c/34$) optimization of Fig. 5, optimized at a taper length $L = 13a$. Vertical axes are exaggerated for scale; topmost (black) figure shows the robust taper design to scale. Even the robust design shows complicated sub-flange oscillations, but similar oscillations are reproduced independent of the parameterization of the taper design during optimization. Top middle (red): robust design using 1024-point linear interpolation (tent functions). Cyan (bottom/right): robust optimization using sine series with successive increase of the number of series terms. 64-term sine series structure (top right) is similar to tent-function (top middle) structure, and is superimposed on the latter as a dotted cyan curve. Nominal optimum (lower left) has even more radical oscillations, designed to create delicate reflection cancellations (which are spoiled by disorder).

The performance of these sine-series designs, shown in Fig. 5(d), is also converging towards the original robust optimum. In fact, the sine series for some L performs *better* with only 4 terms than it does with more terms or with the original tent-function results. It may be, therefore, that the most counter-intuitive feature of the (tent or 64-sine) robust designs, the intra-flange oscillations, are an artifact not of the parameterization but of the model. That is, the optimization is driving the design towards a regime in which the accuracy limitations of CMT and/or the uncertainty model (which cannot accurately capture surface roughness in the context of CMT) are being exploited to reduce reflections in a way that is partially spoiled in practice (e.g. in brute-force calculations or in experiments). Although the robust designs still perform well, and it would not have been feasible to perform optimization of long tapers on a more exact model, these accuracy limitations can be further compensated for by building in *a priori* knowledge of the solution: here, the observation that robust solutions tend to be smooth and slowly oscillatory. (In hindsight, a few-term sine-series basis would have been sufficient to parameterize the robust designs in Fig. 3 and Fig. 4 as well.) Robustness is still required: we have checked that nominal optimization applied to the sine-series parameterization continues to yield significantly worse results. In fact, for the $L = 11a$ 4-term sine-series case where the robust optimum

performed very well, the nominal optimization is immediately trapped in a local minimum and its reflections stay above 10%.

4. Concluding remarks

We have demonstrated how a rapid, semi-analytical Maxwell solver combined with large-scale robust optimization can be used to design taper structures for slow-light photonic-crystal waveguides with performance markedly better than their non-robust counterparts (nominal optima) in the presence of manufacturing variability. In three dimensions, our semi-analytical CMT approach remains feasible [37], and currently seems to be the only feasible computational method in 3d for optimizing the gradual tapers required in slow-light applications. We have shown that robustness, in addition to compensating for manufacturing uncertainty, can also compensate for limitations of CMT to obtain designs that perform well in practice, even though CMT requires increasingly gradual tapers to be accurate as the group velocity decreases. Because we also find that the robust optima tend to be smooth, slowly-oscillating shapes, by building this information into the parameterization *a priori*—parameterizing the shape as a truncated sine series with a few terms—we find that even better results can sometimes be obtained (although robust optimization is still important). (This finding is reminiscent of—but does *not* follow from—our analytical result that smooth shapes, with minimal high-frequency Fourier components of s' , reduce reflections in the asymptotic $L \rightarrow \infty$ limit.) As the group velocity becomes lower, building in smoothness seems to become more and more important for robustness. Using such an *a priori* low-dimensional representation has other potential benefits: combined with the efficiency of CMT it opens the possibility of more expensive *global* optimization approaches. Furthermore, these techniques are easily generalized to taper optimization for other waveguide designs, including in 3d, and other uncertainty models. As robust taper designs are particularly useful for coupling to slow-light modes in realistic experimental settings, they may potentially form a crucial component of complex, reconfigurable and dynamic optomechanical devices.

Acknowledgments

This work was supported in part by the AFOSR MURI for Complex and Robust On-chip Nanophotonics under contract FA9550-09-1-0704 and by the U.S. Army Research Office under contract W911NF-07-D-0004. We are grateful to Professor Bjorn Maes at the University of Mons for assistance with CAMFR. A. Oskooi was supported by a postdoctoral fellowship from the Japan Society for the Promotion of Science (JSPS).