Photonic inverse design for 3-D structures and optical phase change materials

by

Gufan Yin

B.Eng., Tsinghua University (2015)

Submitted to the Department of Materials Science and Engineering in partial fulfillment of the requirements for the degree of Master of Science in Materials Science and Engineering at the MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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Abstract

Advances in materials science and photonic device fabrication techniques have provided great potential for making better photonic devices. For example, 3-D photonic structures can be fabricated, and optical phase change materials can been utilized to make non-volatile reconfigurable multi-state optical components. These advances call for better design methods to fully exploit their potential.

Traditional photonic design methods are inefficient for exploring the full design space because many physical simulations are required and the physical simulations are very time-consuming. Photonic inverse design methods can explore the full design space more efficiently by using the gradient information at the cost of only two physical simulations per iteration.

In this thesis, photonic inverse design algorithms based on the adjoint-variable method have been developed for 3-D structures and optical phase change materials. Ultra-compact waveguide polarization converters with 3-D structures and ultra-compact waveguide switches with optical phase change materials have been designed using such algorithms. Both types of devices have ultra-small footprint and can be designed starting from very simple initial structures. After several hours of optimization, the devices will usually exhibit good performance including low insertion loss and high extinction ratio.

Thesis Supervisor: Juejun Hu
Title: Associate Professor of Materials Science and Engineering
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Chapter 1

Introduction

This chapter introduces the motivation behind this thesis, and explains the importance of inverse design methods by comparing them with other design methods.

1.1 Potential for better photonic devices

Advances in materials science and photonic device fabrication techniques have provided great potential for making better photonic devices. This section introduces two such advances. These advances call for better design methods to fully exploit their potential.

1.1.1 3-D structures

3-D photonic structures can be fabricated by many different methods. For example, 3-D photonic crystals have been fabricated by layer-by-layer deposition and etching [34, 28], layer-by-layer patterning and wafer-fusion [38], self-assembly [3, 63], holographic lithography [6], single diffraction element interference lithography [10], laser chemical vapor deposition [59], and two-photon polymerization [9, 49, 56].

Some of these methods, such as holographic lithography and self-assembly, are usually restricted to fabricating periodic structures. However, most of these methods do not have such restriction. For example, the two-photon polymerization method
focuses two laser beams into a small volume, and the high energy in the focal volume triggers two-photon-initiated polymerization of resins. By scanning the focal point of the two lasers, polymers of arbitrary shapes can be formed. In principle, such methods should be able to fabricate arbitrarily complex 3-D photonic structures.

1.1.2 Optical phase change materials

Phase change materials can be transformed between amorphous phase and crystalline phase in a non-volatile and reversible fashion by applying proper thermal, optical or electrical excitation [62]. For optical phase change materials, the two phases have very different optical properties, such as refractive index and absorption coefficient [62]. Additionally, The phase transition in some phase change materials has multi-level nature, and it can be exploited to create gray-scale patterns by controlling the degree of phase transition [58].

Such excellent properties of optical phase change materials have been utilized for making non-volatile reconfigurable multi-state optical components [61], including metasurfaces [58 13], optical switches based on racetrack resonators [44] and surface plasmon waveguides [45], optoelectronic display [14] and non-volatile multi-level memory [46].

1.2 Design challenges

Traditional photonic design method starts with representing the device structure with a set of parameters, such as width, length, radius, etc. Then the parameters are scanned in some range, and physical simulations are carried out for each device structure represented by some combination of the parameters. The figure of merit of the devices can be calculated from the physical simulations. Good devices are used to refine the scanning range of the parameters, and the above process is iterated until a good enough device is found.

Even though the traditional design method has led to many useful devices in the past, its limitation becomes apparent when designing more advanced devices, such as
those that have arbitrary 3-D structures, or those that need to satisfy multiple design objectives at the same time. For example, with the traditional method, it is very difficult to design a device that can operate at different material phases, at different wavelengths, while having a very small footprint.

The difficulty originates from the fact that each physical simulation is very time consuming, so we can only afford to scan a very small set of parameters. As a result, the actual design space is very limited.

For example, if a planar device is represented by a $20 \times 20$ array, and each element can be 1 or 0 representing whether there is material or not at that position. The full design space has 400 dimensions and has $2^{400} \approx 10^{120}$ devices if we ignore symmetry. If we use the traditional design method and represent the device with 4 parameters, and scan 10 values for each parameter, we can explore $10^4$ devices, which is a very small subset of the full design space.

If the device has full 3-D structure, the full design space is much larger and the actual design space that can be explored is an even smaller subset of the full design space.

1.3 Related methods

How do we explore the full design space? As mentioned above, simple brute force search is unfeasible because each physical simulation takes a long time. Researchers have tried different methods to reduce the search time by cleverly restricting the search space to be a subset of the full design space.

For example, Direct Binary Search method $[51, 64, 29]$ starts with an initial device structure represented by 0 and 1 on a grid. Value 0 denotes there is no material at that position, and value 1 denotes there is material at that position. In each iteration, the search algorithm loops through all the grid points and flips the corresponding value between 0 and 1. A physical simulation is run after each flip of value, and the flipped value is retained if and only if the figure of merit improves after the flip. The above procedure is repeated until the figure of merit cannot be improved. This
method is similar to brute force search because it loops through all the grid points in each iteration, and therefore the number of physical simulations that need to be run in each iteration is the same as the dimension of the design space (400 in the previous $20 \times 20$ array example). It explores a subset of the full design space because the flipped value is only retained if it improves the figure of merit, and this property can let the algorithm be stuck at local optima.

Truncated Newton method [53] calculates the gradient of the figure of merit with respect to all the design parameters by perturbing each design parameter and running a physical simulation after each perturbation. In order to save the time for computing the Hessian matrix, the Hessian matrix is usually simply taken as identity matrix and the method essentially becomes gradient descent method, and then all the design parameters are updated using the gradient to improve the figure of merit. This procedure is repeated until convergence. This method resembles the traditional design method, because the design space can be constructed in the traditional way, e.g., using width, length, radius, etc. It is also related to Direct Binary Search method because the number of physical simulations that need to be run in each iteration is the same as the dimension of the design space.

Another class of methods are based on population, including, e.g., Evolutionary Algorithm [43] and Particle Swarm Optimization [47]. Such methods start with an initial “population” that is a set of different photonic devices in our case. Physical simulations are run for each device in the population to calculate the figure of merit. Then the population is evolved in some way into the next generation of population. The best device is selected after several generations or after the figure of merit does not improve anymore. Different methods in this class differ in the details of how the current generation is evolved into the next. For Evolutionary Algorithm, the population is evolved by selecting good devices, crossover (mixing the parameters of different devices) and mutation (randomly perturb the parameters). For Particle Swarm Optimization, the population is evolved by moving the devices, in parameter space, towards the best device in the population and the best generation in the history of each device.
For these population-based design methods, the number of physical simulations that need to be run in each iteration is the same as the population size, which can be chosen arbitrarily. However, the effective dimension of the design space that can be explored in each iteration is about the size of the population if we do not consider the random perturbation. Fortunately, the space spanned by the population changes after the population evolves to the next generation. Therefore, the effective dimension of the design space that can be eventually reached is greater than the population size. However, in order to efficiently explore the design space, the population size should probably be on the same order of magnitude as the dimension of the design space. In our previous $20 \times 20$ array example, the dimension of the full design space is 400, so the population size should be about hundreds.

Random sampling methods are also used for photonic design. For example, simulated annealing [22] is a Monte Carlo method to explore the design space. This method starts with an initial device and a physical simulation. Then it randomly chooses the next device in the design space according to some probability distribution that is conditioned on the current device, e.g., it can be a Gaussian distribution centered on the current device. A physical simulation is run for the candidate device, and its figure of merit is compared with that of the current device. The candidate device is accepted with some probability, which depends on the figure of merit of the current device and that of the candidate device, and also on the parameter “temperature”. If a candidate device is accepted, it will be used as the device in the next iteration; if it is rejected, the current device will be used in the next iteration. When the candidate device is better than the current device, it is always accepted. When the candidate device is worse than the current device, the probability of accepting it is positively related to the temperature, e.g., by the Boltzmann factor $\exp \left( -\frac{\Delta E}{kT} \right)$, where $\Delta E$ can be the difference in figure of merit, $k$ is constant, $T$ is temperature.

Therefore, when the temperature is high, it is more likely to accept the worse device and continue exploring other areas of the design space; when the temperature is low, it is less likely to accept the worse device and keep using the current device. By slowly decreasing the temperature and sampling enough devices at each temper-
nature, it will likely find an optimal device, for the same reason that annealing can let the materials achieve lower energy state. However, the number of sampling that is required to find the optimal device is usually large, especially in high dimensional design space.

1.4 Inverse design method

For most of the photonic design methods introduced above, the number of physical simulations that need to be run in order to effectively update all the design parameters in an iteration is close to the dimension of the design space, which is 400 in the previous $20 \times 20$ array example. And this is already a large number given that the run time of each physical simulation can range from several minutes to several hours, and typically many iterations are required to find a good design.

Photonic inverse design methods \[19, 33\] can potentially solve this problem and explore the full design space in a more efficient way. Inverse design methods use the gradient of the figure of merit with respect to all the design parameters to optimize all the design variables at the same time. In terms of using gradient, it is similar to the Truncated Newton method introduced above. However, a major difference between them is how the gradient is calculated. Photonic inverse design methods calculate the gradient with respect to all the design parameters using only two physical simulations.

Depending on the function of which the gradient is calculated, there are mainly two types of inverse design methods: adjoint-variable method (also known as topology optimization) \[19\], and objective-first method \[33\].

Both methods start from re-writing the Maxwell equations as a linear equation
of electric field. The Maxwell equations are:

$$\nabla \cdot \mathbf{D} = \rho \quad (1.1)$$
$$\nabla \cdot \mathbf{B} = 0 \quad (1.2)$$
$$\nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J}_{\text{src}} + \sigma \mathbf{E} \quad (1.3)$$
$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad (1.4)$$

The Maxwell equations lead to the following equation for electric field:

$$\nabla \times \mu^{-1} \nabla \times \mathbf{E} + \varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} + \sigma \frac{\partial \mathbf{E}}{\partial t} = -\frac{\partial \mathbf{J}_{\text{src}}}{\partial t} \quad (1.5)$$

where $\mathbf{E}$ is electric field, $\mu$ is permeability, $\varepsilon$ is permittivity, $t$ is time, $\sigma$ is electric conductivity, $\mathbf{J}_{\text{src}}$ is electric current density for the source. If we consider one frequency component of $\mathbf{E}$ and $\mathbf{J}_{\text{src}}$ as $\mathbf{E} e^{-i\omega t}$ and $\mathbf{J}_{\text{src}} e^{-i\omega t}$ respectively, we have

$$\nabla \times \mu^{-1} \nabla \times \mathbf{E} - \varepsilon \omega^2 \mathbf{E} - i\sigma \omega \mathbf{E} = i\omega \mathbf{J}_{\text{src}} \quad (1.6)$$

This is a linear equation of $\mathbf{E}$ and can be rewritten as

$$Ax = b \quad (1.7)$$

where

$$A = \nabla \times \mu^{-1} \nabla \times -\varepsilon(p) \omega^2 - i\sigma \omega \quad (1.8)$$
$$x = \mathbf{E} \quad (1.9)$$
$$b = i\omega \mathbf{J}_{\text{src}} \quad (1.10)$$

and $\varepsilon(p)$ is the parametric representation of $\varepsilon$ by some parameters $p$. 
1.4.1 Adjoint-variable method

Adjoint-variable method was originally developed for optimizing the shape of mechanical structures [2] and was later applied to optimize photonic devices [37, 19, 25, 36, 42, 18, 17, 35, 55, 52]. It uses the gradient of the design objective function to update the design variables. The design objective function $F(x, p)$ is defined to represent our design objective that we want to minimize. In case the function needs to be maximized, we can simply multiply $F$ by $-1$ and minimize it as usual. Such a function can include requirements on the electric field $x$ and on the parameters $p$ for imposing fabrication constraints. If $F$ is differentiable as in Wirtinger Calculus, then we can optimize the structure $p$ based on the differential

$$\frac{dF}{dp} = 2\text{Re} \left( \frac{\partial F}{\partial x} \frac{\partial x}{\partial p} \right) + \frac{\partial F}{\partial p} (1.11)$$

where the Wirtinger derivative is defined as

$$\frac{\partial F}{\partial x} = \frac{1}{2} \left( \frac{\partial F}{\partial \text{Re}(x)} - i \frac{\partial F}{\partial \text{Im}(x)} \right) (1.12)$$

$\frac{\partial F}{\partial x}$ and $\frac{\partial F}{\partial p}$ are readily available from our definition of $F$. $\frac{\partial x}{\partial p}$ can be obtained by taking derivative of Equation (1.7) with respect to $p$:

$$\frac{\partial x}{\partial p} = A^{-1} \left( \frac{\partial b}{\partial p} - x^T \partial A^T \frac{\partial p}{\partial p} \right) (1.13)$$

where $\frac{\partial b}{\partial p}$ is usually zero and $\frac{\partial A}{\partial p}$ is easy to calculate because the operator $A$ is constructed using the parameterization of the permittivity $\epsilon(p)$. Then Equation (1.11) can be written as

$$\frac{dF}{dp} = 2\text{Re} \left\{ \frac{\partial F}{\partial x} A^{-1} \left( \frac{\partial b}{\partial p} - x^T \partial A^T \frac{\partial p}{\partial p} \right) \right\} + \frac{\partial F}{\partial p} (1.14)$$

However, the matrix $A$ is usually ill-conditioned and difficult to inverse directly. The adjoint-variable method avoids directly inverting $A$ by constructing another linear
such that the “adjoint field” $y$ can be solved in the same way as how the electric field $x$ is solved in physical simulation. Because

$$y^T = \frac{\partial F}{\partial x} A^{-1}$$

we have the differential

$$\frac{dF}{dp} = 2 \text{Re} \left\{ y^T \left( \frac{\partial b}{\partial p} - x^T \frac{\partial A^T}{\partial p} \right) \right\} + \frac{\partial F}{\partial p}$$

and we can update $p$ iteratively to minimize $F$:

$$p_{k+1} = p_k - s \frac{dF}{dp_k}$$

where $k$ is the iteration number and $s$ is the step size.

In this way, we can optimize all the parameters in $p$ at the same time in each iteration at the expense of two physical simulations — one for solving the electric field $x$, and the other for solving the adjoint field $y$. Therefore, the full design space can in principle be explored much more efficiently.

### 1.4.2 Objective-first method

Objective-first method [33, 32, 30, 31, 41, 4, 5] sets the desired electric field as hard constraints. As expected, Maxwell equations cannot be satisfied given the initial device structure and these hard constraints on the electric field. How far is the system from satisfying the Maxwell equations is described by the physical residual:

$$L(x, p) = |A(p)x - b|^2$$

where $A, x, p, b$ have the same meaning as in Equation (1.7).
Then the gradient of the physical residual $L$ is used to update $x$ and $p$ in order to minimize $L$. In the ideal case, if $L$ can be minimized to zero, we will have a device that can perfectly satisfy our design objectives and the Maxwell equations. If we imposed some constraints on the electric field that are impossible to realize, or our optimization method is not good enough, $L$ cannot be minimized to zero. Empirical studies show that if $L$ can be reduced to some small enough value, then we will have a device that can satisfy our design objectives reasonably well.

Directly minimizing $L$ with respect to the two variables $x$ and $p$ is challenging because there is a term where they are multiplied together. Fortunately, $L$ is easy to minimize with respect to each variable separately. First, $L$ is convex with respect to $x$, which can be easily optimized using standard convex optimization method. And if the parametric representation of permittivity $\epsilon(p)$ is linear with respect to $p$, as it is in the case of using the full design space, then $L$ is convex with respect to $p$ as well. Therefore $L$ is usually minimized with respect to the two variables alternately and iteratively in practice.

In this way, we can optimize all the parameters in $p$ at the same time in each iteration at the expense of two passes of minimization per iteration — one for minimizing $L$ with respect to the electric field $x$, and the other for minimizing $L$ with respect to $p$. Therefore, the full design space can in principle be explored much more efficiently.

1.4.3 Comparison

There are some similarities between the adjoint-variable method and the objective-first method. First of all, they can both efficiently optimize all the design variables in each iteration based on the gradient information. However, they also share the same challenge. The gradient information is local by definition, so they will both result in local optima rather than global optima. Therefore, the initial condition and the optimization scheme are very important for the success of these methods.

They are different in that they use gradients of different functions to update the design variables. The adjoint-variable method uses the gradient of the design objective function, and the objective-first method uses the gradient of the physical residual.
Chapter 2

3-D structures

2.1 Optimization problem

In the following application, we will use adjoint-variable method to design the photonic devices. The design objective is to maximize the power of a particular waveguide mode at the output port. The normalized power of \( m \)-th mode \( S_m \) and the power at the output port \( S_{\text{out}} \) are

\[
S_m = \int E_m \times H_m^* \cdot dn \tag{2.1}
\]

\[
S_{\text{out}} = \int E \times H^* \cdot dn \tag{2.2}
\]

where \( E_m \) is the electric field for \( m \)-th mode, \( H_m \) is the magnetic field for the \( m \)-th mode, \( E \) is the electric field at the output port, \( H \) is the magnetic field at the output port. The power at the output port that is contributed by the \( m \)-th mode can be derived using the orthogonality of guided modes [35], and the result is

\[
P_m = \frac{1}{4} \left| \frac{\int E \times H_m^* \cdot dn}{S_m} + \frac{\int E_m^* \times H \cdot dn}{S_m^*} \right|^2 \text{Re}(S_m) \tag{2.3}
\]

The magnetic field \( H \) in \( P_m \) can be calculated from electric field \( E \) using Maxwell equations:

\[
H = \frac{i}{\mu \omega} \nabla \times E \tag{2.4}
\]
Therefore, the objective function that needs to be minimized can be written as the negative power of $m$-th waveguide mode $F(x) = -P_m$ where $x$ denotes the electric field. The optimization problem is

$$\begin{align*}
\text{minimize} & \quad F(x) \\
\text{subject to} & \quad Ax = b \\
& \quad 0 \leq p \leq 1
\end{align*}$$

(2.5)

where

$$A = \nabla \times \mu^{-1} \nabla \times -\epsilon(p)\omega^2 - i\sigma\omega$$

(2.8)

$$b = i\omega J_{\text{src}}$$

(2.9)

as introduced in Chapter [1]. The current source $J_{\text{src}}$ is determined by the input waveguide mode. $\epsilon$ is parameterized by $p \in [0, 1]^N$ where each dimension of $p$ corresponds to a voxel in the design region, and $N$ is the total number of voxels in the design region. The explicit equation for this parameterization is

$$\epsilon(p) = \epsilon_{\min} + (\epsilon_{\max} - \epsilon_{\min})p$$

(2.10)

where $\epsilon_{\min}$ and $\epsilon_{\max}$ are the lower bound and upper bound of the allowed permittivity value in the design region respectively. In the rest of the thesis, $\epsilon$ will be used to denote relative permittivity $\epsilon_r = \epsilon/\epsilon_0$, and the subscript $r$ will be omitted to avoid cluttering of notation.

During optimization, the gradient $\frac{dF}{dp}$ is normalized to have modulus 1, and the step size for updating $p$ is $s = 0.001$. 

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2.2 Waveguide polarization converter

2.2.1 Introduction

In photonic integrated circuits, the photonic devices usually exhibit different properties for light with different polarizations. This problem is more severe in high-index-contrast devices because the high index contrast makes the difference between boundary conditions for different polarizations more pronounced. Therefore, it is useful to be able to convert the polarization of light in photonic integrated circuits [1].

Polarization converters utilizing periodic perturbation of waveguide cross section [50], different propagation constants for orthogonal modes in asymmetric waveguides [16, 21, 57, 65, 40, 7, 15], adiabatic mode evolution [60, 11, 8] and genetic algorithm [66] have been demonstrated. Most of these polarization converters have length of tens or hundreds of micrometers for silicon waveguide and light with wavelength 1.55 µm. The most compact one has length 2 µm and uses triangular waveguides to convert the polarization [65].

Here we use the adjoint-variable method to design 3-D waveguide polarization converters with even smaller footprint.

2.2.2 Device design

The material is silicon with refractive index $n = 3.5$ ($\epsilon_{\text{max}} = 12.25$), surrounded by air with refractive index $n = 1$ ($\epsilon_{\text{min}} = 1$). The operating wavelength is 1.55 µm. The resolution is 0.05 µm. The waveguide is parallel to $x$ direction. The cross section of the waveguide has dimension 0.4 µm × 0.4 µm. The design region has dimension 1 µm × 0.4 µm × 0.4 µm. The input waveguide mode (Fig. 2-1) is TM$_{00}$ mode with the electric field mainly along $z$ direction, and the target waveguide mode (Fig. 2-2) is TE$_{00}$ mode with the electric field mainly along $y$ direction.

The initial device structure is chosen to be $p = 0.6$ for all the voxels, i.e., $\epsilon = 7.75$. The initial $\epsilon$, $E_y$ and $E_z$ are shown in Fig. 2-3. The physical simulation is carried out using the Finite Difference Time Domain (FDTD) method in the software MEEP [39].
We can see that the initial device structure has very high insertion loss due to the large index mismatch between the design region and the input/output ports.

The permittivity and the electric field after 5 and 19 iterations are shown in Fig. 2-4 and Fig. 2-6 respectively. The 3-D visualizations of the structures are shown in Fig. 2-5 and Fig. 2-7 respectively. The threshold for showing the structure in the 3-D visualization is chosen to be $p \geq 0.5$, i.e., $\epsilon \geq 6.625$. 

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We can see that the algorithm automatically fills in the device structure in the design region without any human input. After 5 iterations, the device structure has some coarse features as shown in Fig. 2-5. After 19 iterations, device structure has finer features as shown in Fig. 2-7. The optimized device structure does not look very intuitive, and seems to be some diagonal structure in the cross section perpendicular to $x$. It is likely that the operating principle is similar to those asymmetric waveguide structures introduced above.

Figure 2-4: The permittivity for $p = 0.6$ and the electric field at the cross section perpendicular to $z$ at half thickness after 5 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-5: 3-D visualization of the device structure after 5 iterations of optimization. The threshold for showing the structure is $p \geq 0.5$, i.e., $\epsilon \geq 6.625$.

During optimization, the output port has more $E_y$ component and less $E_z$ component, indicating that the TM input mode has been converted to TE mode. Mode match integral shows that the output port has 92.0% ($-0.36$ dB) of input power in
Figure 2-6: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 19 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-7: 3-D visualization of the device structure after 19 iterations of optimization. The threshold for showing the structure is $p \geq 0.5$, i.e., $\epsilon \geq 6.625$.

the target mode (TE$_{00}$ mode), and 2.0% ($-17.0$ dB) of the input power in the input mode (TM$_{00}$ mode). The power and the extinction ratio of the two modes during optimization are shown in Fig. 2-8. The extinction ratio is defined as

$$10 \log \frac{P_{\text{target}}}{P_{\text{input}}}$$

where $P_{\text{target}}$ and $P_{\text{input}}$ are the power of target mode and input mode at the output port respectively. The extinction ratio exceeds $20$ dB during optimization, and is $16.6$ dB for the final device optimized for the output power of the target mode.

Each iteration of optimization takes less than 3 minutes on a typical desktop computer, and the whole optimization process with 19 iterations and 38 physical simulations can be finished within one hour.
Figure 2-8: The power and the extinction ratio of the target and input mode during optimization.

2.2.3 Different initial permittivity

The same optimization process has been applied to devices with different initial permittivity, e.g., $p = 0.2 \ (\epsilon = 3.25)$ and $p = 1 \ (\epsilon = 12.25)$.

The initial permittivity and the electric field for $p = 0.2 \ (\epsilon = 3.25)$ are shown in Fig. 2-9. The permittivity and the electric field after 36 iterations of optimization are shown in Fig. 2-10. The 3-D visualization of the structure is shown in Fig. 2-11. The power and the extinction ratio of the two modes during optimization is shown in Fig. 2-12. For the optimized device, the output port has 91.8% ($-0.37 \text{ dB}$) of input power in the target mode (TE$_{00}$ mode), and 2.5% ($-16.0 \text{ dB}$) of the input power in the input mode (TM$_{00}$ mode). The extinction ratio is 15.6 dB for the final device.
Figure 2-9: The initial permittivity for $p = 0.2$ and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-10: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 36 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-11: 3-D visualization of the device structure after 36 iterations of optimization. The threshold for showing the structure is $p \geq 0.5$, i.e., $\epsilon \geq 6.625$. 

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Figure 2-12: The power and the extinction ratio of the target and input mode during optimization.
The initial permittivity and the electric field for \( p = 1 \) \( (\epsilon = 12.25) \) are shown in Fig. 2-13. The permittivity and the electric field after 22 iterations of optimization are shown in Fig. 2-14. The 3-D visualization of the structure is shown in Fig. 2-15. The power and the extinction ratio of the two modes during optimization is shown in Fig. 2-16. For the optimized device, the output port has 91.8\% \((-0.37\, \text{dB})\) of input power in the target mode (\( \text{TE}_{00} \) mode), and 1.9\% \((-17.2\, \text{dB})\) of the input power in the input mode (\( \text{TM}_{00} \) mode). The extinction ratio is 16.8\, \text{dB} for the final device.

Figure 2-13: The initial permittivity for \( p = 1 \) and the electric field calculated from FDTD simulation at the cross section perpendicular to \( z \) at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-14: The permittivity and the electric field at the cross section perpendicular to \( z \) at half thickness after 22 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Surprisingly, devices with different initial permittivity lead to very similar optimized device structures and performance (Table 2.1), although the performance during optimization is different for the devices with different initial permittivity.
Figure 2-15: 3-D visualization of the device structure after 22 iterations of optimization. The threshold for showing the structure is $p \geq 0.5$, i.e., $\epsilon \geq 6.625$.

Figure 2-16: The power and the extinction ratio of the target and input mode during optimization.

Table 2.1: Performance of optimized devices starting from different initial structures

<table>
<thead>
<tr>
<th>$p$</th>
<th>Conversion efficiency (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>91.8</td>
<td>15.6</td>
</tr>
<tr>
<td>0.6</td>
<td>92.0</td>
<td>16.6</td>
</tr>
<tr>
<td>1</td>
<td>91.8</td>
<td>16.8</td>
</tr>
</tbody>
</table>
2.2.4 Different device size

The same optimization process has been applied to devices with a larger size, 2 µm × 1 µm × 0.4 µm. And different initial device permittivity is used, e.g., \( p = 0.2 (\epsilon = 3.25) \), \( p = 0.6 (\epsilon = 7.75) \) and \( p = 1 (\epsilon = 12.25) \). The optimization results for \( p = 0.2 \) are shown in Fig. 2-17, Fig. 2-18, Fig. 2-19 and Fig. 2-20. The optimization results for \( p = 0.6 \) are shown in Fig. 2-21, Fig. 2-22, Fig. 2-23 and Fig. 2-24. The optimization results for \( p = 1 \) are shown in Fig. 2-25, Fig. 2-26, Fig. 2-27 and Fig. 2-28.

Figure 2-17: The initial permittivity for \( p = 0.2 \) and the electric field calculated from FDTD simulation at the cross section perpendicular to \( z \) at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-18: The permittivity and the electric field at the cross section perpendicular to \( z \) at half thickness after 40 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

It can be seen that devices with different initial permittivity lead to very different optimized device structures and performance (Table 2.2). In this case, the device size is larger than that in previous section. The reason why devices with different initial permittivity lead to different optimized device structures in this case can be
Figure 2-19: 3-D visualization of the device structure after 40 iterations of optimization. The threshold for showing the structure is $p \geq 0.5$, i.e., $\epsilon \geq 6.625$.

Figure 2-20: The power and the extinction ratio of the target and input mode during optimization.

interpreted as follows. When the device size is larger, the design space is larger, the optimization landscape is more complex and there are more local optima. Because the adjoint-variable method is based on gradient information, which is local information by definition. Therefore, it can be easily “stuck” in some local optimum, and where it gets “stuck” depends on where it starts. When the algorithm starts with different initial device permittivity, it will find the local optimum structure approachable from that initial structure, and such local optimum structures are likely to be different when the design space is large with complex optimization landscape.
Figure 2-21: The initial permittivity for $p = 0.6$ and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-22: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 27 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Table 2.2: Performance of optimized devices with size $2 \mu m \times 1 \mu m \times 0.4 \mu m$ starting from different initial structures

<table>
<thead>
<tr>
<th>$p$</th>
<th>Conversion efficiency (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>97.4</td>
<td>19.6</td>
</tr>
<tr>
<td>0.6</td>
<td>87.8</td>
<td>20.7</td>
</tr>
<tr>
<td>1</td>
<td>84.3</td>
<td>18.1</td>
</tr>
</tbody>
</table>
Figure 2-23: 3-D visualization of the device structure after 27 iterations of optimization. The threshold for showing the structure is $p \geq 0.5$, i.e., $\epsilon \geq 6.625$.

Figure 2-24: The power and the extinction ratio of the target and input mode during optimization.

Figure 2-25: The initial permittivity for $p = 1$ and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.
Figure 2-26: The permittivity and the electric field at the cross section perpendicular to \( z \) at half thickness after 21 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-27: 3-D visualization of the device structure after 21 iterations of optimization. The threshold for showing the structure is \( p \geq 0.5 \), i.e., \( \epsilon \geq 6.625 \).

Figure 2-28: The power and the extinction ratio of the target and input mode during optimization.
Smaller device sizes have also been tried using the same optimization process. An example with size \(0.5 \mu m \times 0.4 \mu m \times 0.4 \mu m\) starting from \(p = 0.6\) (\(\epsilon = 7.75\)) can be seen in Fig. 2-29, Fig. 2-30, Fig. 2-31 and Fig. 2-32. We can see that the optimized device structure is similar to those with size \(1 \mu m \times 0.4 \mu m \times 0.4 \mu m\) because the design space is smaller and simpler for smaller devices, so the algorithm finds similar local optimum structures. However, the performance of the smaller device is not good, with conversion efficiency 66.2\% and extinction ratio 3.9 dB. It is likely to be limited by the laws of physics and might provide an upper bound of the performance for such small devices.

![Figure 2-29](image1)

Figure 2-29: The initial permittivity for \(p = 0.6\) and the electric field calculated from FDTD simulation at the cross section perpendicular to \(z\) at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

![Figure 2-30](image2)

Figure 2-30: The permittivity and the electric field at the cross section perpendicular to \(z\) at half thickness after 12 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.
Figure 2-31: 3-D visualization of the device structure after 12 iterations of optimization. The threshold for showing the structure is $p \geq 0.5$, i.e., $\epsilon \geq 6.625$.

Figure 2-32: The power and the extinction ratio of the target and input mode during optimization.

### 2.2.5 Different index contrast

The same optimization process has been applied to devices with a different refractive index contrast. Instead of silicon with refractive index 3.5, silicon nitride with refractive index 2.0 is used for the devices that are surrounded by air with refractive index 1.0. Due to the small index contrast, smaller devices can no longer provide good performance. Device with size $2 \mu m \times 0.8 \mu m \times 0.8 \mu m$ starting from $p = 0.6$ ($\epsilon = 2.8$) is shown in Fig. 2-33, Fig. 2-34, Fig. 2-35 and Fig. 2-36. Device with size $2 \mu m \times 2 \mu m \times 0.8 \mu m$ starting from $p = 0.6$ ($\epsilon = 2.8$) is shown in Fig. 2-37, Fig. 2-38.
Figure 2-33: The initial permittivity for $p = 0.6$ and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-34: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 25 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

The performance of the two devices with small index contrast is summarized in Table 2.3. They perform worse than devices with a large index contrast. It suggests the importance of large index contrast in achieving good performance with compact photonic devices.

There is another point that is worth noting. The device with larger size $2\, \mu m \times 2\, \mu m \times 0.8\, \mu m$ performs worse than the device with smaller size $2\, \mu m \times 0.8\, \mu m \times 0.8\, \mu m$. Theoretically speaking, the larger device has a larger design space that is a superset of the design space for the smaller device, so the optimal device with a larger size
cannot be worse than that with a smaller size. However, the difficulty in optimization dominates in this case. Even though the larger device can potentially achieve a better optimized structure, it is sometimes difficult to find an initial structure or optimization method that can actually achieve that optimized structure. This problem is more severe for larger devices because they have larger design space with more complex optimization landscape. A potential solution might be to use the optimized device with a smaller size as the initial device structure for optimizing the device with a larger size.
Figure 2-37: The initial permittivity for \( p = 0.6 \) and the electric field calculated from FDTD simulation at the cross section perpendicular to \( z \) at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 2-38: The permittivity and the electric field at the cross section perpendicular to \( z \) at half thickness after 40 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

<table>
<thead>
<tr>
<th>Size ( (\mu \text{m}) )</th>
<th>Conversion efficiency (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 2 \times 0.8 \times 0.8 )</td>
<td>72.6</td>
<td>5.7</td>
</tr>
<tr>
<td>( 2 \times 2 \times 0.8 )</td>
<td>51.3</td>
<td>4.2</td>
</tr>
</tbody>
</table>
Figure 2-39: 3-D visualization of the device structure after 40 iterations of optimization. The threshold for showing the structure is $p \geq 0.5$, i.e., $\epsilon \geq 2.5$.

Figure 2-40: The power and the extinction ratio of the target and input mode during optimization.
Chapter 3

Optical phase change materials

3.1 Optimization problem

The formulation of the optimization problem in Chapter 2 can be easily extended to multi-objective optimization problems. For example, different objective functions $F_i(x)$ can be defined for devices with different material phases, output ports, modes and wavelength, etc. The actual objective function for the optimization problem is thus

$$F(x) = \sum_i \alpha_i F_i(x)$$

(3.1)

where $\alpha_i$ are the weights for different objective functions $F_i(x)$, and they can be tuned to emphasize some design objectives.

3.2 Waveguide switch

3.2.1 Introduction

Photonic waveguide switches are important for realizing photonic integrated circuits [23]. Waveguide switches have been realized or proposed using electro-optic effect [68, 24], thermo-optic effect [12] and phase change materials [18, 44, 20, 26, 27, 54, 67]. The advantages of using phase change materials include [61] 1) they can provide large change in refractive index between different phases that can enable
compact device structure, and 2) they can enable non-volatile switches that do not require continuous power supply.

Waveguide switches using phase change materials are usually based on controlling the optical path length in Mach-Zehnder Interferometers [18, 20, 27], controlling the resonant frequency and quality factor of resonators [44, 54], controlling the absorption in the waveguide [20], or controlling the coupling condition by controlling the mode profiles [67].

Here we use the adjoint-variable method to design compact waveguide switches based on phase change materials with planar structures.

### 3.2.2 Device design

The material is Ge$_2$Sb$_2$Se$_4$Te$_1$ with refractive index $n_a = 3.33$ in amorphous phase and $n_c = 5.08 + 0.35i$ in crystalline phase, i.e., $\epsilon_a = 11.1$ and $\epsilon_c = 25.7 + 3.6i$. The imaginary part of the refractive index corresponds to the optical loss in the material. The operating wavelength is 1.55 $\mu$m. The resolution is 0.04 $\mu$m. The waveguide is parallel to $x$ direction. The cross section of the waveguide has dimension 0.4 $\mu$m $\times$ 0.4 $\mu$m. The design region with phase change material has dimension 2 $\mu$m $\times$ 2 $\mu$m $\times$ 0.4 $\mu$m and can be switched between the amorphous phase and the crystalline phase. The waveguide for the input port and the two output ports are fixed to be in the amorphous phase. The input waveguide mode and the target waveguide mode are both TE$_{00}$ mode with the electric field mainly along $y$ direction.

When the phase change material is in the amorphous phase, the output power of the mode in the upper branch is maximized, and that in the lower branch is minimized. When the phase change material is in the crystalline phase, the output power of the mode in the upper branch is minimized, and that in the lower branch is maximized. More formally, the objective function that we want to minimize is

$$F(x) = -P_{a,1} + P_{a,2} + P_{c,1} - P_{c,2}$$  \hspace{1cm} (3.2)

where $a$ stands for amorphous, $c$ for crystalline, 1 for the output port in the upper
branch, and 2 for the output port in the lower branch.

The initial device structure is chosen to be a “V” shape in the design region with \( p = 0.6 \) \((\epsilon_a = 7.1\) for amorphous phase and \(\epsilon_c = 15.8 + 2.1i\) for crystalline phase\). The real part of the initial \(\epsilon\) and \(E_y\) for both amorphous phase and crystalline phase are shown in Fig. 3-1. The physical simulation is carried out using the Finite Difference Time Domain (FDTD) method in the software MEEP [39]. Because the device structure is symmetrical with respect to the plane \(y = 0\), the output power is equally divided between the two output ports.

![Figure 3-1: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to \(z\) at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.](image)

(a) \(\epsilon\) in amorphous phase  (b) \(E_y\) in amorphous phase

(c) \(\epsilon\) in crystalline phase  (d) \(E_y\) in crystalline phase

The permittivity and the electric field after 40 iterations are shown in Fig. 3-2. When the phase change material is in the amorphous phase, the output power is 80.8\% in port 1, and 0.12\% in port 2. The extinction ratio between the two ports is 28.3. When the phase change material is in the crystalline phase, the output power is 0.037\% in port 1, and 81.3\% in port 2. The extinction ratio between the two ports is 33.4. The performance of the device is summarized in Table 3.1. The performance
during optimization is shown in Fig. 3-3.

![Image](a) $\epsilon$ in amorphous phase (b) $E_y$ in amorphous phase

![Image](c) $\epsilon$ in crystalline phase (d) $E_y$ in crystalline phase

Figure 3-2: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 40 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>80.8</td>
<td>0.12</td>
<td>28.3</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.037</td>
<td>81.3</td>
<td>33.4</td>
</tr>
</tbody>
</table>

Table 3.1: Output power and extinction ratio of the waveguide switch

3.2.3 Different initial permittivity

The same optimization process has been applied to devices with different initial permittivity, e.g., $p = 0.2$ ($\epsilon_a = 3.0$ for amorphous phase, $\epsilon_c = 5.9 + 0.7i$ for crystalline phase) and $p = 1$ ($\epsilon_a = 11.1$ for amorphous phase, $\epsilon_c = 25.7+3.6$ for crystalline phase). The design region with phase change material has dimension $2\mu m \times 2\mu m \times 0.4\mu m$.

For $p = 0.2$, the initial permittivity and electric field are shown in Fig. 3-4. The structure and electric field after 38 iterations of optimization are shown in Fig. 3-5.
The performance of the device is summarized in Table 3.2. The performance during optimization is shown in Fig. 3-6.

We can see that if we start with $p = 0.2$, the optimized device cannot achieve our goal. No matter the phase change material is in amorphous phase or crystalline phase, there is always more output power in port 2 (lower branch) than port 1 (upper branch). The reason might be that the initial permittivity in the design region is so low that the light is not well confined. And the gradient calculated from the adjoint-variable method is related to the electric field. Therefore, the gradient cannot effectively optimize the device performance. This problem is more severe for the amorphous phase because the permittivity is even lower in amorphous phase and the light is worse confined. As a result, the device seems be optimized only for the crystalline phase and there is always more output power in port 2 no matter which phase the material is in.

Table 3.2: Output power and extinction ratio of the waveguide switch

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>5.1</td>
<td>7.6</td>
<td>-1.7</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.33</td>
<td>71.3</td>
<td>23.3</td>
</tr>
</tbody>
</table>
Figure 3-4: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 3-5: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 38 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.
Figure 3-6: The power and the extinction ratio of the two output ports during optimization.
For $p = 1$, the initial structure and electric field are shown in Fig. 3-7. The structure and electric field after 41 iterations of optimization are shown in Fig. 3-8. The performance of the device is summarized in Table 3.3. The performance during optimization is shown in Fig. 3-9. In this case, the performance of the optimized device is reasonable. However, the insertion loss for the crystalline phase is much higher than that for the amorphous phase.

![Images](a) $\epsilon$ in amorphous phase (b) $E_y$ in amorphous phase

![Images](c) $\epsilon$ in crystalline phase (d) $E_y$ in crystalline phase

Figure 3-7: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Table 3.3: Output power and extinction ratio of the waveguide switch

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>78.1</td>
<td>0.30</td>
<td>24.2</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.28</td>
<td>58.7</td>
<td>23.2</td>
</tr>
</tbody>
</table>
Figure 3-8: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 41 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 3-9: The power and the extinction ratio of the two output ports during optimization.
3.2.4 Different weight coefficient

As is shown in the previous section, the performance of the optimized device when the material is in one phase might be much worse than in the other phase. In order to address this problem, different weight coefficients $\alpha_i$ are used. The coefficients $\alpha_i$ give different weights to different objective functions as in

$$F(x) = \sum_i \alpha_i F_i(x)$$  \hspace{1cm} (3.3)

For example, we use the following objective function for initial parameter $p = 0.2$.

$$F(x) = -2P_{a,1} + 2P_{a,2} + P_{c,1} - P_{c,2}$$  \hspace{1cm} (3.4)

The design region with phase change material has dimension 2 $\mu$m $\times$ 2 $\mu$m $\times$ 0.4 $\mu$m. The initial structure and electric field are shown in Fig. 3-10. The structure and electric field after 32 iterations of optimization are shown in Fig. 3-11. The performance of the device is summarized in Table 3.4. The performance during optimization is shown in Fig. 3-12. We can see that the optimized device has much better performance compared with the one also starting with $p = 0.2$ but using the same weights for all the design objectives.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>68.7</td>
<td>3.1</td>
<td>13.5</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.71</td>
<td>67.7</td>
<td>19.8</td>
</tr>
</tbody>
</table>
Figure 3-10: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to \( z \) at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 3-11: The permittivity and the electric field at the cross section perpendicular to \( z \) at half thickness after 32 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.
Figure 3-12: The power and the extinction ratio of the two output ports during optimization.
To further test the method of changing weight coefficients, we use the following objective function for $p = 1$.

$$F(x) = -P_{a,1} + P_{a,2} + 2P_{c,1} - 2P_{c,2}$$

(3.5)

The initial structure and electric field are shown in Fig. 3-13. The structure and electric field after 29 iterations of optimization are shown in Fig. 3-14. The performance of the device is summarized in Table 3.5. The performance during optimization is shown in Fig. 3-15. We can see that the optimized device has much more balanced performance for the two phases compared with the one also starting with $p = 1$ but using the same weights for all the design objectives.

Figure 3-13: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.
Figure 3-14: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 29 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Table 3.5: Output power and extinction ratio of the waveguide switch

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>70.4</td>
<td>1.0</td>
<td>18.5</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.71</td>
<td>66.8</td>
<td>19.7</td>
</tr>
</tbody>
</table>

Figure 3-15: The power and the extinction ratio of the two output ports during optimization.
3.2.5 Different initial structure

The same optimization process has been applied to devices with different initial structures, e.g., triangle and square. The design region with phase change material has dimension $2 \mu m \times 2 \mu m \times 0.4 \mu m$.

For the device with initial structure of a triangle and $p = 0.6$ ($\epsilon_a = 7.1$ for amorphous phase and $\epsilon_c = 15.8 + 2.1i$ for crystalline phase), the real part of the initial permittivity and electric field are shown in Fig. 3-16. The permittivity and the electric field after 20 iterations are shown in Fig. 3-17. The performance of the device is summarized in Table 3.6. The performance during optimization is shown in Fig. 3-18. The performance of this optimized device is worse than that of the optimized device with initial structure being “V” shape, but the performance is still reasonable.

(a) $\epsilon$ in amorphous phase  (b) $E_y$ in amorphous phase

(c) $\epsilon$ in crystalline phase  (d) $E_y$ in crystalline phase

Figure 3-16: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.
Figure 3-17: The permittivity and the electric field at the cross section perpendicular to \( z \) at half thickness after 20 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Table 3.6: Output power and extinction ratio of the waveguide switch

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>66.3</td>
<td>0.79</td>
<td>19.2</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.73</td>
<td>62.9</td>
<td>19.4</td>
</tr>
</tbody>
</table>

Figure 3-18: The power and the extinction ratio of the two output ports during optimization.
For the device with initial structure of a square and \( p = 0.6 \) (\( \epsilon_a = 7.1 \) for amorphous phase and \( \epsilon_c = 15.8 + 2.1i \) for crystalline phase), the real part of the initial permittivity and electric field are shown in Fig. 3-19. The permittivity and the electric field after 24 iterations are shown in Fig. 3-20. The performance of the device is summarized in Table 3.7. The performance during optimization is shown in Fig. 3-21. The performance of this optimized device is worse than that of the optimized device with initial structure being “V” shape, but the performance is still reasonable and comparable to that starting with the triangle structure.

![Figure 3-19: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to \( z \) at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.](image)

![Figure 3-20: The permittivity and the electric field after 24 iterations.](image)

**Table 3.7: Output power and extinction ratio of the waveguide switch**

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>75.4</td>
<td>0.78</td>
<td>19.9</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.50</td>
<td>51.8</td>
<td>20.2</td>
</tr>
</tbody>
</table>

By starting from different simple initial structures, the algorithm can always find the device structures that perform reasonable well after only tens of iterations of
optimization. This demonstrates the power of the algorithm. However, as we can see from the results of the optimization, the boundaries of the optimized structures are similar to the initial structures, and are thus different for different initial structures. This indicates that the optimization landscape for this problem is complex enough such that the algorithm has been stuck at some local optimum that can only provide reasonable, but not great, performance.
3.2.6 Different device size

Devices with a smaller size (1 µm × 2 µm × 0.4 µm) have also been investigated.

For \( p = 0.2 \), the initial structure and electric field are shown in Fig. 3-22. The structure and electric field after 40 iterations of optimization are shown in Fig. 3-23. The performance of the device is summarized in Table 3.8. The performance during optimization is shown in Fig. 3-24.

We can see that if we start with \( p = 0.2 \), the optimized device cannot achieve our goal. No matter the phase change material is in amorphous phase or crystalline phase, there is always more output power in port 2 (lower branch) than port 1 (upper branch). It is similar to the case where \( p = 0.2 \) and the device size is larger (2 µm × 2 µm × 0.4 µm). We attribute this problem to the same reason as is explained in the case of larger devices.

Table 3.8: Output power and extinction ratio of the waveguide switch

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>4.9</td>
<td>7.4</td>
<td>-1.8</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.40</td>
<td>57.3</td>
<td>21.6</td>
</tr>
</tbody>
</table>
Figure 3-22: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.
Figure 3-23: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 40 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 3-24: The power and the extinction ratio of the two output ports during optimization.
For $p = 0.6$, the initial structure and electric field are shown in Fig. 3-25. The structure and electric field after 40 iterations of optimization are shown in Fig. 3-26. The performance of the device is summarized in Table 3.9. The performance during optimization is shown in Fig. 3-27. In this case, the extinction ratio of the optimized device is reasonable, but the insertion loss for the amorphous phase is very high.

![Figure 3-25: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.](image)

![Figure 3-26: The real part of the permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.](image)

Table 3.9: Output power and extinction ratio of the waveguide switch

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>35.3</td>
<td>2.6</td>
<td>11.3</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.31</td>
<td>63.1</td>
<td>23.1</td>
</tr>
</tbody>
</table>
(a) $\epsilon$ in amorphous phase  (b) $E_y$ in amorphous phase  

(c) $\epsilon$ in crystalline phase  (d) $E_y$ in crystalline phase

Figure 3-26: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 40 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

(a) Power  

(b) Extinction ratio

Figure 3-27: The power and the extinction ratio of the two output ports during optimization.
For $p = 1$, the initial structure and electric field are shown in Fig. 3-28. The structure and electric field after 20 iterations of optimization are shown in Fig. 3-29. The performance of the device is summarized in Table 3.10. The performance during optimization is shown in Fig. 3-30. In this case, the performance of the optimized device is reasonable.

Figure 3-28: The real part of the initial permittivity and the electric field calculated from FDTD simulation at the cross section perpendicular to $z$ at half thickness. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Table 3.10: Output power and extinction ratio of the waveguide switch

<table>
<thead>
<tr>
<th>Phase</th>
<th>Power in port 1 (%)</th>
<th>Power in port 2 (%)</th>
<th>Extinction ratio (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amorphous</td>
<td>55.1</td>
<td>2.8</td>
<td>12.9</td>
</tr>
<tr>
<td>Crystalline</td>
<td>0.66</td>
<td>53.2</td>
<td>19.1</td>
</tr>
</tbody>
</table>
Figure 3-29: The permittivity and the electric field at the cross section perpendicular to $z$ at half thickness after 20 iterations of optimization. The input port of the waveguide is on the left. The color map for the electric field is in arbitrary unit.

Figure 3-30: The power and the extinction ratio of the two output ports during optimization.
Chapter 4

Summary and outlook

In this thesis, photonic inverse design algorithms based on the adjoint-variable method have been developed for 3-D structures and optical phase change materials. Ultra-compact waveguide polarization converters with 3-D structures and ultra-compact waveguide switch with optical phase change materials have been designed using such algorithms. Both types of devices have ultra-small footprint and can be designed starting from very simple initial structures. After several hours of optimization, the devices will usually exhibit good performance including low insertion loss and high extinction ratio.

The main advantage of such algorithms is that all the design variables, e.g., the permittivity for all the voxels in the design region, can be optimized using the gradient information at the cost of only two physical simulations per iteration. Therefore, these algorithms have the potential to explore the full design space more efficiently and to design better devices with unintuitive structures that are hard to design with traditional methods.

However, the main limitation of these algorithms is that they rely on the gradient information, which is local information by definition. Therefore, when they arrive at some local optima, the gradient will vanish and it will be difficult for the algorithms to escape from the local optima. Such local optima may not necessarily correspond to devices with good performance. Whether or not such local optima have good performance depends on the optimization landscape, the initial condition and
the optimization method. When the algorithms start with different permittivity or different structures, they may find very different optimized devices with very different performance if the optimization landscapes are complex enough.

To address this limitation, it might be necessary to combine the inverse design algorithms and other traditional optimization algorithms. For example, the population-based optimization algorithms or random sampling algorithms can be used to search the space of “initial conditions” and other hyperparameters, and the inverse design algorithms can be used to find the local optima that can be reached from those initial conditions. In this way, we can benefit from the best of both methods — the global property of traditional optimization algorithms for escaping from local optima, and the local property of inverse design algorithms for efficient local optimization.

Another limitation is that the optimization is carried out with continuous variables, so the permittivity of a voxel can have some value between the background and the device material. After binarizing the structure to be 0 or 1 based on some threshold, the device performance will drop. One method to address this limitation is to parameterize the boundary of the structure, and optimize the boundary instead of the permittivity for each voxel.

Despite the limitations, photonic inverse design methods can complement traditional design methods to design better photonic devices while unlocking the potential of the advances in photonic device fabrication techniques and materials science.
Bibliography


