Adjoint Method Supported Topology Optimization for Electromagnetic/Photonic Inverse Design

Ergun Simsek, Sumya H. Oishe, and Raonaqul Islam
University of Maryland Baltimore County, Baltimore, MD 21250, USA

***Abstract*—Topology optimization is a powerful computational approach for designing photonic and electromagnetic structures by optimizing material distribution within a given domain. In this study, we explore novel applications of adjoint-based topology optimization, including enhanced substrate design for two-dimensional materials, improved quantum efficiency in photodetectors, and a photonic medium for real-time object classification. We demonstrate a substrate optimization method that increases the absorption of broadband excitations in monolayer MoS_2 by 72% and boosts quantum efficiency by 141%. Additionally, we introduce an optimized photonic medium that classifies objects at the speed of light by manipulating wavefront propagation.**

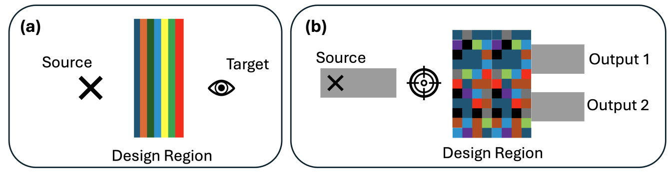

Fig. 1. (a) 1D and (b) 2D inverse design problems. The former seeks a multilayered substrate leading to the strongest field intensity at the observation point. The latter aims to determine the permittivity array that leads to input pulse to a different port depending on the target type.

I. Introduction

Topology optimization is a computational design methodology that systematically determines the optimal material distribution within a predefined design space to achieve a desired performance objective while satisfying physical and manufacturing constraints [1]. This approach, which relies on numerical techniques such as gradient-based optimization and level-set methods, has been widely utilized in structural mechanics and has seen exponential growth in applications within electromagnetics and photonics over the past two decades. The work of Georgieva *et al.* [2] represents one of the earliest demonstrations of the feasibility of adjoint sensitivity techniques for electromagnetic design optimization, establishing a foundation for their application in photonics. A decade later, Jensen and Sigmund's review [1] captured the rapid advancements in topology optimization for nanophotonics, where the adjoint method was employed to design structures such as photonic crystals, waveguides, and resonators. The pixel-based parameterization of geometry enabled unprecedented design flexibility and efficiency, leading to innovative developments in subsequent years, including optical cloaking [3], mode conversion [4], and beam splitting based on wavelength [4], [5], polarization [4], or power [4]. Additional breakthroughs included the design of fiber couplers [4] and photonic fibers [6]. In this paper, we present novel applications of topology optimization, including substrate design [7] with layered medium Green's functions [8], improving the quantum efficiency of a photodetector [9], and designing a medium for object classification using light [10].

II. Topology vs Adjoint Optimization

In photonic/electromagnetic inverse design, the topology optimization enables the identification of the permittivity distribution that maximizes or minimizes a specific objective function, such as field intensity at a target point or efficient wave routing. Figure 1 illustrates two cases: (a) A one-dimensional (1D) design where a multilayered substrate is optimized to achieve maximum field intensity at an observation point; (b) a two-dimensional (2D) design where a pixelated permittivity distribution is optimized to guide an input pulse to different output ports depending on the target type.

For both problems, we define an objective function $F(\varepsilon)$ that depends on the permittivity distribution ε in the design domain. The optimization problem is formulated as $\max_\varepsilon F(\varepsilon)$, subject to physical constraints such as Maxwell's equations, ensuring wave propagation follows physical laws $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$ and $\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$, where $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic fields, and $\mathbf{D}$ and $\mathbf{B}$ are the electric displacement and magnetic flux density. Additionally, material constraints impose that the permittivity values remain within a predefined range, typically expressed as $\varepsilon_{\text{min}} \leq \varepsilon \leq \varepsilon_{\text{max}}$.

Adjoint optimization is used to efficiently compute the gradient of the objective function with respect to permittivity changes, enabling rapid updates to the design. The sensitivity of $F(\varepsilon)$ to a small perturbation in permittivity $\delta\varepsilon$ is computed as:

$$\frac{\partial F}{\partial \varepsilon} = -\Re\left(\mathbf{E}^\dagger \cdot \frac{\partial A}{\partial \varepsilon}\mathbf{E}\right), \tag{1}$$

where A is the system matrix from the discretized Maxwell equations, $\mathbf{E}$ is the forward field solution, and $\mathbf{E}^\dagger$ is the adjoint field solution, obtained by solving a second Maxwell's equation with a different source term. Using the computed gradient $\frac{\partial F}{\partial \varepsilon}$, the permittivity distribution is updated iteratively using methods such as gradient-based optimization. At each iteration, the permittivity values are adjusted to improve the objective function until convergence.

III. Numerical Results

A. Substrate Optimization

Over the past two decades, research on 2D materials like MoS_2 and graphene has grown significantly. Typically, we use

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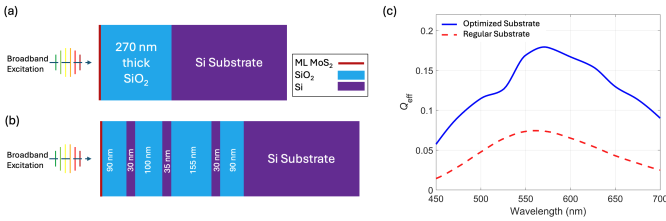

Fig. 2. Monolayer MoS_2 on (a) a 270 nm SiO_2/Si substrate, (b) an optimized substrate under broadband illumination, and (c) quantum efficiency of MoS_2-based phototransistors for regular and optimized substrates at 10 V gate voltage, 0.5 V source-drain voltage, and 0.2 μW incidence power.

SiO_2-coated Si substrates with 90 nm or 270 nm thicknesses, as shown in Fig. 2 (a). We aim to optimize substrate design using the adjoint method to maximize contrast under broadband excitation given the constraint of using SiO_2 and Si thin films only.

We assume the plane-wave excitation has a broadband spectrum (400–750 nm, peak at 575 nm) and MoS_2's thickness is 0.65 nm. We use 1000 inner layers (1 nm each) in the adjoint optimization, initially all SiO_2. Iteratively, each layer is set to Si if $\partial F/\partial \epsilon_r$ exceeds the average; otherwise, remaining SiO_2. The inverse design converges in 88 iterations, yielding four SiO_2/Si pairs of varying thicknesses as shown in Fig. 2 (b). To validate the design, we compute power at MoS_2's center using an FDFD solver, showing a 72% enhancement compared the 270 nm thick SiO_2 substrate. Next, we assess the quantum efficiency of MoS_2-based phototransistors. These devices, with metal contacts on monolayer MoS_2 over a SiO_2/Si substrate, convert optical excitations into current, with efficiency determined via drift-diffusion simulations [11]. Fig. 2 (c) shows quantum efficiency as a function of excitation wavelength: 7.5% at 561 nm for a 270 nm SiO_2 substrate, rising to 18% at 571 nm with the optimized design—a 141% peak increase and 210% average enhancement.

B. Object Classification

We employ the adjoint method for topology optimization to design a photonic medium capable of classifying two distinct objects at the speed of light. The computational domain consists of an input waveguide, a design region, and two output ports, as depicted in Figs. 3 (a) and (b). The topology optimization algorithm iteratively adjusts the material distribution within the design region to ensure that light exits from different ports depending on the object's shape. Without a scatterer, the light propagates through the middle port, while the presence of a "0"- or "1"-shaped scatterer alters the wavefront, directing the light towards distinct output channels, as demonstrated in Figs. 3 (c) and (d). By dynamically training the system with variations of each object class, we ensure robustness against slight shape variations. The designed medium enables real-time optical object classification without needing electronic processing, making it a promising avenue for ultrafast computing and sensing applications.

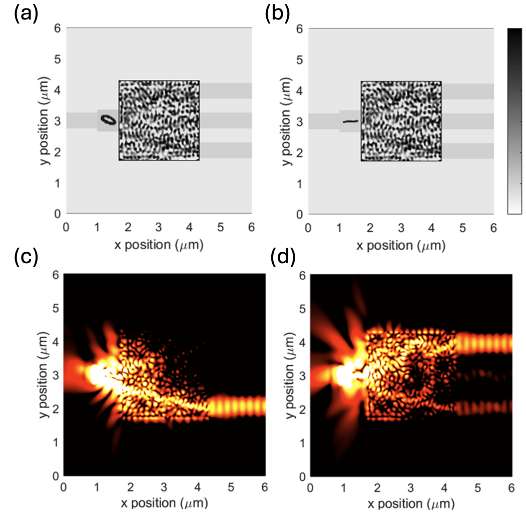

Fig. 3. (a) and (b) illustrate the computation domain with a zero- and one-shaped scatter, respectively; (c) and (d) show how light propagates through different ports and achieves object classification. When there is no scatterer, the light exits from the middle port.

IV. Conclusion

Our research confirms that topology optimization, combined with adjoint sensitivity analysis, provides a powerful framework for designing both electromagnetic and photonic structures and devices. More detailed case studies will be presented at the conference.

References

[1] J. S. Jensen and O. Sigmund, "Topology optimization for nanophotonics," *Laser Photonics Rev.*, vol. 5, no. 2, pp. 308–321, 2011.

[2] N. K. Georgieva, S. Glavic, M. H. Bakr, and J. W. Bandler, "Feasible adjoint sensitivity technique for EM design optimization," *IEEE Trans. Microw. Theory Tech.*, vol. 50, no. 12, pp. 2751–2758, 2002.

[3] O. D. Miller, "Photonic design: From fundamental solar cell physics to computational inverse design," Ph.D. dissertation, University of California, Berkeley, 2012, doctoral dissertation.

[4] J. Lu and J. Vučković, "Nanophotonic computational design," *Optics Express*, vol. 21, no. 11, pp. 13 351–13 367, 2013.

[5] A. Y. Piggott *et al.*, "Inverse design and demonstration of a compact and broadband on-chip wavelength demultiplexer," *Nature Photonics*, vol. 9, no. 6, pp. 374–377, 2015.

[6] C. Sitawarin, W. Jin, Z. Lin, and A. W. Rodriguez, "Inverse-designed photonic fibers and metasurfaces for nonlinear frequency conversion," *Photonics Research*, vol. 6, no. 5, pp. B82–B88, 2018.

[7] S. H. Oishe, R. Islam, C. R. Menyuk, and E. Simsek, "Broadband substrate optimization with adjoint method and Green's functions," in *International Photonic Conference (IPC)*. IEEE, 2024.

[8] E. Simsek, Q. H. Liu, and B. Wei, "Singularity subtraction for evaluation of Green's functions for multilayer media," *IEEE Trans. Microw. Theory Tech.*, vol. 54, no. 1, pp. 216–225, 2006.

[9] E. Simsek, R. Islam, S. H. Oishe, and C. R. Menyuk, "Substrate optimization with the adjoint method and layered medium Green's functions," *JOSA B*, vol. 41, no. 10, pp. 2259–2265, 2024.

[10] E. Simsek and S. H. Oishe, "A multi-objective permittivity optimization for object classification at the speed of light," *Machine Learning: Science and Technology*, 2025. [Online]. Available: http://iopscience.iop.org/article/10.1088/2632-2153/ae139b

[11] R. Islam *et al.*, "Study of an MoS_2 phototransistor using a compact numerical method enabling detailed analysis of 2D material phototransistors," *Scientific Reports*, vol. 14, no. 1, p. 15269, 2024.