

# Substrate Optimization with Adjoint Method and Layered Medium Green's Functions

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**Abstract:** In recent years, the photonics community has shown increasing interest in the inverse design of photonic components and devices using the adjoint method (AM) due to its efficient gradient computation and suitability for large parameter and continuous design spaces. This work focuses on substrate optimization to maximize light transmission or field enhancement at specific locations using layered medium Green's functions (LMGFs). We first provide a numerical formulation for calculating two-dimensional (2D) LMGFs, leveraging their efficiency for fixed sources and observation points parallel to layer interfaces. We then present a step-by-step implementation of the AM for substrate optimization using LMGFs. Through numerical studies, we verify the field enhancement achieved with AM-designed substrates using a frequency-domain solver. We compare the results of AM with particle swarm optimization (PSO) for two optimization problems, demonstrating that AM not only generates realistic designs with smooth permittivity profiles but also achieves inverse design more efficiently than PSO. The AM designs are easier to fabricate and require significantly less computational effort due to the efficient gradient computation inherent in the method. This study underscores the advantages of AM in designing photonic devices with continuous parameter spaces.

## 1. Introduction

In the last decade, there has been growing interest in the photonics community in the inverse design of photonic components and devices using the adjoint method (AM) [1–13]. This choice has several advantages over other modern numerical optimization techniques, such as particle swarm optimization (PSO) [10, 14–16] and the genetic algorithm (GA) [10, 14, 17]. First, AM provides efficient computation of gradients with respect to design parameters with a computational cost that is independent of the number of design parameters. This unique property of AM is particularly advantageous in optimization problems where the number of design parameters is large. Second, AM is well-suited for problems with continuous design spaces, where the design parameters can take on any real value within user-determined limits. GA and PSO, on the other hand, face challenges in handling continuous design spaces, especially if the number of parameters to be optimized is large, e.g., as the number of parameters increases in a PSO implementation, the search space expands exponentially, making it harder for the swarm to explore effectively and find optimal solutions. This leads to sparse sampling and slower convergence since particles take longer to locate promising regions. Additionally, the risk of premature convergence to sub-optimal solutions rises, complicating the optimization process. The fitness landscape in high-dimensional spaces is more complex, with numerous local optima and steep gradients, making navigation through this space and global optimization difficult.

Substrate optimization for maximizing the transmission of light through the substrate or maximizing the field at a specific location at a desired wavelength or wavelength range typically involves designing the properties of the substrate material, such as the permittivity and thickness [11–13, 18–26]. It is known that stacks of thin films with varying refractive indices and coatings with a gradually changing refractive index can reduce reflections, and AM has already been utilized to design substrates [11, 12]. In those studies [11, 12], researchers have used either the

47 frequency-domain finite differences (FDFD), time-domain finite differences (FDTD), or the  
 48 transfer-matrix method. Here, we achieve the same goal using layered medium Green's functions  
 49 (LMGFs).

50 For a multi-layered planar geometry, LMGFs give us the electric and magnetic fields created  
 51 by electrical or magnetic dipoles or line sources placed at any location in that multi-layered  
 52 geometry [27–30]. As discussed later, the LMGF formulation requires less computation time  
 53 for the solution if the computation makes use of the following fact: For a fixed source, if the  
 54 coordinates of observation points change parallel to the layer interfaces, then one needs to  
 55 calculate the spectral domain LMGFs only once, and their spatial counterparts can be computed  
 56 via adaptive integration all at once.

57 The outline of this paper is as follows. We first provide a complete formulation to calculate the  
 58 two-dimensional (2D) LMGFs numerically. Then we provide a step-by-step recipe to implement  
 59 an adjoint method for substrate optimization using LMGFs. In the numerical results section, we  
 60 verify the field enhancement that is achieved with substrates that are designed with the adjoint  
 61 method using a frequency-domain finite-differences (FDFD) solver for two different optimization  
 62 problems and conclude.

## 63 2. Evaluation of 2D LMGFs

64 Previously, we followed the formulation developed by Chew [27] to calculate the LMGFs for  
 65 line [28] and dipole [29] sources. Both studies reduced computation time by subtracting the  
 66 singularities from the spectral domain LMGFs and adding their contributions to the spatial domain  
 67 using some Bessel and Hankel function formulae. Here, we follow the recursive formulation  
 68 developed initially for anisotropic medium LMGFs [30] as follows.

69 Figure 1 illustrates a medium with  $N + 1$  layers aligned parallel to the  $x$ -axis, where each layer  
 70 is defined with its electrical permittivity ( $\epsilon_\ell = \epsilon_0 \epsilon_{r,\ell}$ ), magnetic permeability ( $\mu_\ell = \mu_0 \mu_{r,\ell}$ ),  
 71 thickness ( $h_\ell$ ) for  $\ell = 0, 1, \dots, N$ , and  $h_0 = h_{N+1} = \infty$ , and  $\epsilon_0$  and  $\mu_0$  are the electrical  
 72 permittivity and magnetic permeability of vacuum. The infinitely long source parallel to the  
 73  $y$ -axis is located at  $(x', z')$  in layer- $m$ . The wavenumber in layer- $\ell$  is  $k_\ell^2 = \omega^2 \epsilon_\ell \mu_\ell$ , where  
 74  $\omega = 2\pi f$  and  $f$  is the frequency of the electromagnetic waves created by the line source. The  
 75 electric field at the observation point  $(x, z)$ , which can be chosen in any layer, can be determined  
 76 by evaluating the following Sommerfeld integral

$$E_y(x, z|x', z') = \frac{1}{4\pi k_\ell} \int_0^\infty \left\{ \tilde{G}(x, z|x', z') \frac{\cos(k_x|x-x'|)}{k_z} \right\} dk_x, \quad (1)$$

77 where  $\tilde{G}(x, z|x', z')$  is the spectral domain LMGF that can be calculated with

$$\tilde{G}(x, z|x', z') = \Phi_\ell e^{u_\ell(z-z_i)} + \Psi_\ell e^{-u_\ell(z-z_{i-1})}, \quad (2)$$

78 where  $\Phi_\ell$  and  $\Psi_\ell$  are unknowns that need to be determined according to continuity conditions of  
 79 the electric and magnetic fields at the interfaces,  $k_x$  is the integration variable,  $k_{z,\ell}^2 + k_x^2 = k_\ell^2$ ,  
 80 and  $u_\ell = jk_{z,\ell}$ . When the source is in the bottom layer ( $m = 0$ ), then  $\Psi_0 = 0$ , and similarly,  
 81 when the source is in the top layer ( $m = N + 1$ ), then  $\Phi_{N+1} = 0$ . By imposing the boundary  
 82 conditions for electric and magnetic fields, we can create a linear equation to determine all these  
 83 coefficients, i.e.,  $\mathbf{A}\mathbf{X} = \mathbf{S}$ , where  $\mathbf{A} \in C^{2N \times 2N}$ ,  $\mathbf{X} \in C^{2N}$ , and  $\mathbf{S} \in S^{2N}$ . The non-zero elements  
 84 of  $\mathbf{A}$  are provided in the Appendix section. To construct the vector  $\mathbf{X}$ , we set

$$\begin{aligned} x_1 &= \Phi_0, \quad x_{2n} = \Psi_N, \\ x_{2i} &= \Phi_i, \quad x_{2i+1} = \Psi_i, \end{aligned} \quad (3)$$

85 for  $i = 1, \dots, N - 1$ .

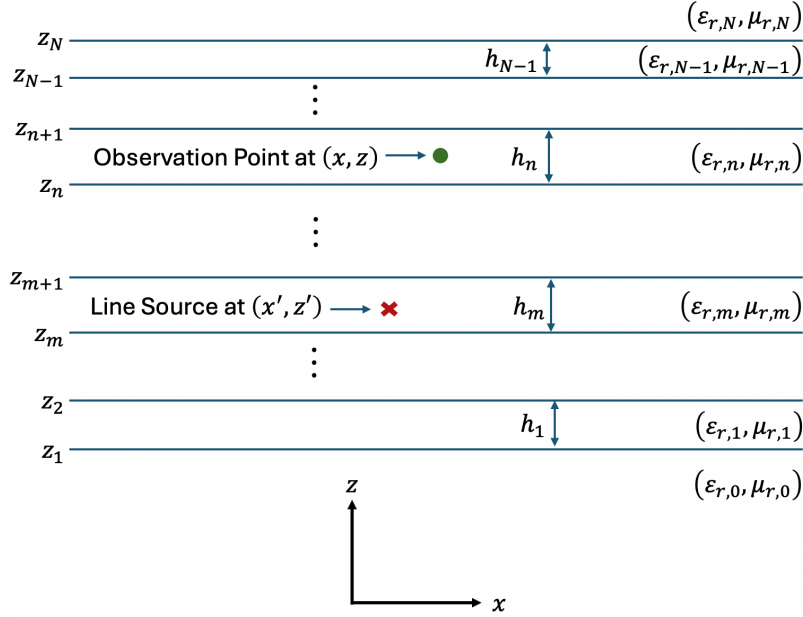


Fig. 1. Schematic illustration of a multilayered medium with  $N + 1$  layers and  $N$  interfaces parallel to  $x$ -axis. The thickness of layer- $\ell$  is  $h_\ell$ . The relative electrical permittivity and magnetic permeability of the material used in layer- $\ell$  are  $\epsilon_{r,\ell}$  and  $\mu_{r,\ell}$ , respectively.

86 To construct the vector  $\mathbf{S}$ , we set

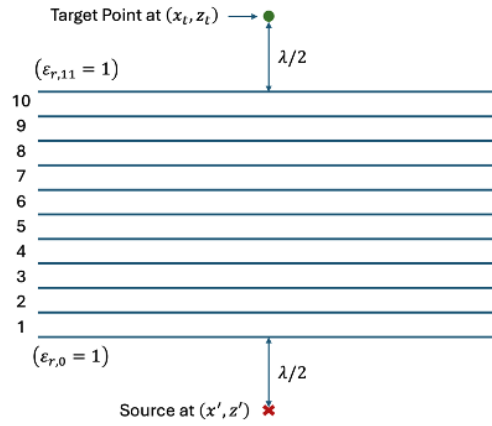
$$\begin{aligned} S_{2j-1} &= \frac{e^{-u_j|z_{j-1}-z'|}}{u_j}, & S_{2j} &= \frac{e^{-u_j|z_{j-1}-z'|}}{\epsilon_j}, \\ S_{2j+1} &= -\frac{e^{-u_j|z_j-z'|}}{u_j}, & S_{2j+2} &= \frac{e^{-u_j|z_j-z'|}}{\epsilon_j}. \end{aligned} \quad (4)$$

87 If in (4), the source is in the bottom layer, i.e.,  $m = 0$ , we then set  $S_{2m-1} = 0$  and  $S_{2m} = 0$ .  
88 Similarly, if the source is in the top layer  $m = n$ , we then set  $S_{2m+1} = 0$  and  $S_{2m+2} = 0$ .  
89 After determining the unknown coefficients, we numerically compute Eq. (1) using a 32-point  
90 Gauss-Legendre quadrature. It is essential to note that when the source location is fixed and  
91 observation points have the same  $z$  coordinate but different  $x$  values, we must calculate the  
92 spectral domain LMGFs only once. Hence, evaluating Eq. (1) for  $n_d$  observations on an axis  
93 parallel to  $\hat{x}$ , we calculate all the LMGFs in a single run, reducing the computation time by  
94 almost  $n_d$  times compared to evaluating them one by one.

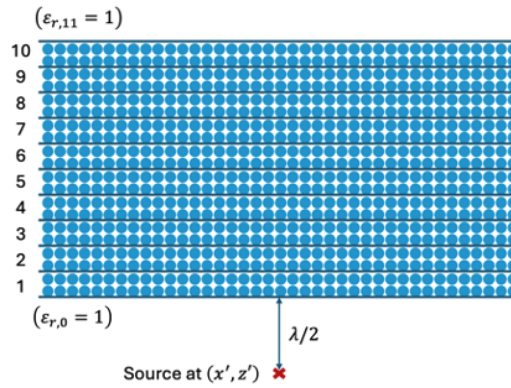
### 95 3. Implementation of Adjoint Method with LMGFs

96 We start with the following simple example to describe how the adjoint method can be implemented  
97 with 2D LMGFs. Assume that we have a  $2\lambda$  thick substrate between  $z = -2\lambda$  and  $z = 0$ . A line  
98 source is at  $(x' = 0, z' = -2.5\lambda)$ , half wavelength below the substrate. Our goal is to design a  
99 substrate that would yield the highest electric field at  $(x_t = 0, z_t = 0.5\lambda)$ , half wavelength above  
100 the substrate. For the sake of simplicity, let us assume that the substrate consists of 10 layers  
101 with the same layer thickness ( $\lambda/5$ ), as shown in Fig. 2 (a). Assuming all the materials are  
102 non-magnetic, we aim to determine each layer's permittivity using the AM.

(a) Step-1



(b) Step-2



(c) Step-3:

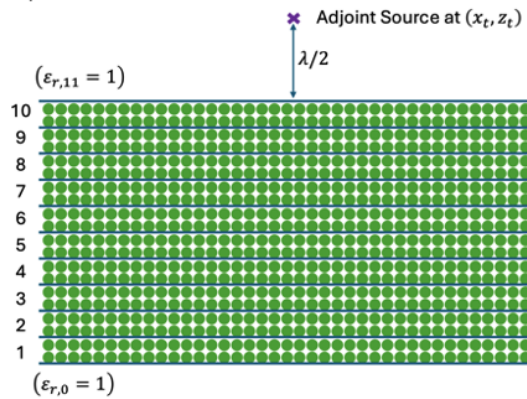


Fig. 2. Schematic illustrations of (a) target, (b) forward, and (c) backward field calculations where small circles and crosses represent field and source points, respectively.

103 As explained in [2–9, 11], the AM requires only two computations to calculate the gradients  
104 with respect to the design parameters. For this problem, we choose our cost function ( $\vartheta$ ) in order

105 to maximize the electric field intensity ( $|E|^2$ ) at the target location  $(x_t, z_t)$  and use the following  
 106 equation to calculate the gradient

$$\frac{\partial \vartheta}{\partial \epsilon_{r,\ell}} = -2k_0^2 \sum_d \text{Re} \left\{ E_\ell^{\text{forw}} \cdot E_\ell^{\text{adj}} \right\} \quad (5)$$

107 where  $E_\ell^{\text{forw}}$  is the electric field created by the original line source and calculated at  $d$  observation  
 108 points located in layer- $\ell$  as shown in Figs. 2 (b) and  $E_\ell^{\text{adj}}$  is the adjoint field calculated at the  
 109 same observation points due to an adjoint source located at the target position as shown in Figs.  
 110 2 (c). Analogically, if  $E_\ell^{\text{forw}}$  is the value that we obtain with Eq. (1) when there is a line source at  
 111  $(x', z')$  carrying 1 A of current, then the  $E_\ell^{\text{adj}}$  is the value we obtain from the same equation for  
 112 a line source at  $(x_t, z_t)$  carrying a complex current of  $2jE^*(x_t, y_t|x', z')/\omega$  A, where  $E^*$  is the  
 113 complex conjugate of  $E$ . In other words, our adjoint field at an observation point  $(x_d, y_d)$  is

$$E^{\text{adj}} = \frac{2j}{\omega} E^*(x_t, z_t|x', z') E_\ell^{\text{back}}(x_d, z_d|x_t, z_t). \quad (6)$$

114 where  $E_\ell^{\text{back}}(x_d, z_d|x_t, z_t)$  is the value that we obtain with Eq. (1) when there is a line source at  
 115  $(x_t, z_t)$  carrying 1 A of current.

116 Our iterative implementation has five steps that can be formulated as follows.

- 117 • Step-1: Calculate the electric field  $E(x_t, y_t|x', y')$  at the target point where we want to  
 118 enhance the electric field as shown in Fig. 2 (a).
- 119 • Step-2: Calculate the electric field  $E_\ell^{\text{forw}}(x_d, z_d|x', z')$  at observation points that cover  
 120 a wide range horizontally (e.g.,  $-4\lambda \leq x \leq 4\lambda$ ) and dense enough vertically (e.g., 20  
 121 observation points per wavelength) inside each layer, as illustrated in Fig. 2 (b).
- 122 • Step-3: Repeat Step-2 by changing the source location with the target location, i.e.,  
 123 calculate  $E_\ell^{\text{back}}(x_d, z_d|x_t, z_t)$ , as depicted in Fig. 2 (c).
- 124 • Step-4: Update the permittivity of each layer using Eqs. (5) and (7).

$$\epsilon_{r,\ell}^{\text{new}} = \epsilon_{r,\ell}^{\text{current}} + \alpha \frac{\partial \vartheta}{\partial \epsilon_{r,\ell}} \quad (7)$$

125 where  $\alpha$  is the learning rate,  $\epsilon_{r,\ell}^{\text{current}}$  is the relative electrical permittivity of layer- $\ell$  used in  
 126 the current set of calculations, and  $\epsilon_{r,\ell}^{\text{new}}$  is the updated permittivity to be used in the next  
 127 iteration.

- 128 • Step 5: Calculate  $\sum_\ell |\partial \vartheta / \partial \epsilon_{r,\ell}|$ . If it is smaller than the desired threshold value, stop  
 129 iterating. Otherwise, go back to Step-1.

130 Note that using symmetry properties of LMGFs (e.g.  $E_y(x, z|x', z') = -E_y(-x, z|x', z')$ ),  
 131 vectorial evaluation of numerical integration, and parallel computing, the computation time  
 132 of steps 2 and 3 can be reduced significantly. Also, if we would like to achieve broadband  
 133 optimization, then we can update the permittivity of each layer as follows. Let's assume, we  
 134 have  $K$  discrete values representing the spectrum of interest where the intensity of the light at  
 135 wavelength- $\zeta$  is  $I_\zeta$  for  $\zeta = 1, 2, \dots, K$ . Then the permittivity of layer- $\ell$  can be computed by

$$\epsilon_{r,\ell}^{\text{new}} = \epsilon_{r,\ell}^{\text{current}} + \frac{\alpha}{K} \sum_{\zeta=1}^K I_\zeta \frac{\partial \vartheta_\zeta}{\partial \epsilon_{r,\ell}}. \quad (8)$$

136 **4. Numerical Results**

137 For all the examples presented here, the learning rate ( $\alpha$ ) is set to 0.05.

138 **4.1. Permittivity Optimization**

139 We first start with the aforementioned simple optimization problem. Assume the wavelength of  
 140 the electromagnetic waves created by the line source is 600 nm, and we are trying to determine  
 141 the permittivity values of each layer of the substrate,  $\epsilon_{r,\ell}$  for  $\ell = 1, 2, \dots, 10$ . The top and  
 142 bottom layers are both air ( $\epsilon_{r,0} = \epsilon_{r,11} = 1$ ). As a design constraint, we enforce  $1 \leq \epsilon_{r,\ell} \leq 4$ .  
 143 For the first iteration of the optimization process, we set  $\epsilon_{r,\ell} = 2$  for all  $\ell$ .

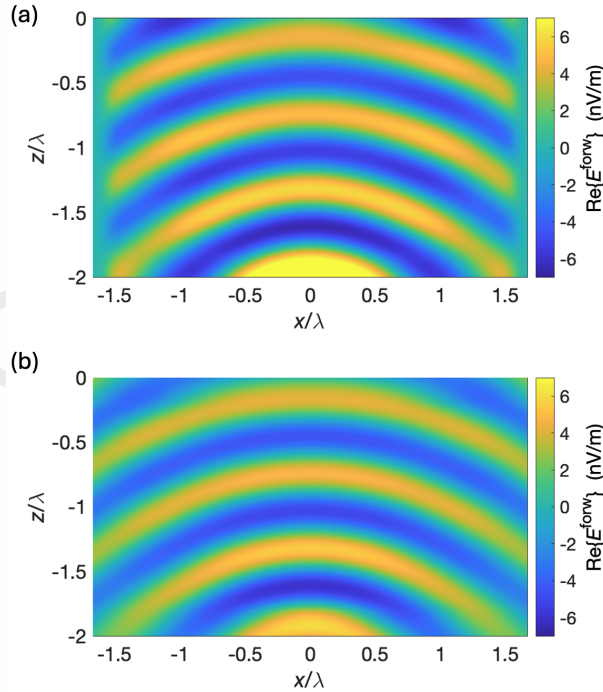


Fig. 3. Real part of the electric field ( $E^{\text{forw}}$ ) for the forward calculation obtained using (a) an FDFD solver and (b) LMGFs.

144 To validate the accuracy of our LMGF implementation, we calculate the electric field values  
 145 along the substrate using our LMGF formulation and an FDFD solver. For the FDFD solution,  
 146 we set the unit mesh length to 5 nm. Similarly, for the LMGF implementation, we create a grid in  
 147 each layer with a grid step length of 5 nm (horizontally and vertically) for  $-1\mu\text{m} \leq x \leq 1\mu\text{m}$ . In  
 148 Fig. 3, we plot the electric field's real part only for brevity. Due to the perfectly matched layers  
 149 (PML) on both sides of the substrates, the results obtained with the FDFD gradually decrease in  
 150 those PML regions. Apart from those regions, the results look almost identical.

151 For the first AM-based substrate optimization example, we assume the same geometry explained  
 152 at the beginning of the previous section, e.g., the substrate is  $2\lambda$  thick from  $z = -2\lambda$  to  $z = 0$ , the  
 153 line source is at  $x' = 0$  and  $z' = -2.5\lambda$ , and the substrate consists of ten  $\lambda/5$ -thick layers. We  
 154 continue to use 20 points per wavelength sampling density, hence there are 640 target points in  
 155 each layer, i.e., 4 points vertically and 160 points horizontally. With the selected design constraint  
 156 and initial permittivity values, the AM implemented with the LMGF formalism generates a design,  
 157 as depicted by the blue line in Fig. 4, which yields an 11.1% increase compared to a glass

158 slide with a relative permittivity of 2.25 (corresponding to the refractive index of 1.5), which  
 159 is the typical value for the permittivity of optical glass substrates. We also implement another  
 160 numerical optimization method using the PSO method. Using 100 swarms and 300 iterations,  
 161 the PSO recommends a similar but slightly different design, shown with the red dashed lines in  
 162 Fig. 4, which yields an 11.13% increase compared to the glass slide. Note that we obtain much  
 163 more significant enhancements by increasing the maximum electrical permittivity allowed from  
 164 4 to a higher value, e.g., 20. However, since our primary focus is the applicability of the AM  
 165 method for one-dimensional problems such as substrate optimization using LMGFs, we do not  
 166 discuss those cases here.

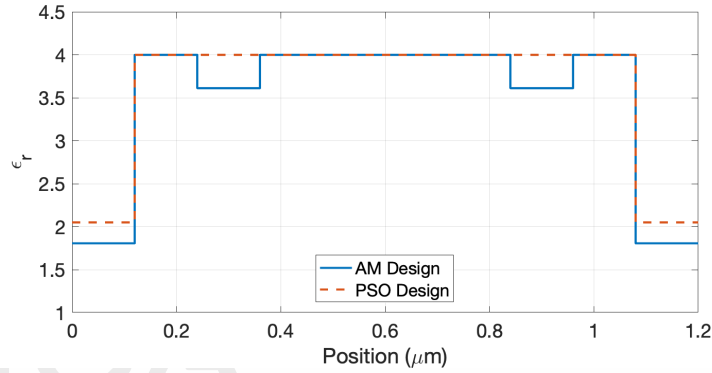


Fig. 4. Solid and dashed lines show the optimized permittivity values along the AM and PSO designed substrates with 10 thin layers that lead to an 11.09 % and an 11.13% enhancement, respectively.

167 For the second set of substrate optimization studies, we increase the number of layers within  
 168 the substrate to 240 and follow the same procedure. Since these are  $\lambda/120$ -thick layers, we have  
 169 160 target points in each layer. For the initial step, we set all the relative permittivity values  
 170 to 2.0 for all 240 thin layers. The PSO implementation uses 2400 swarms, with the maximum  
 171 number of iterations set to 1000, but the computation ends nearly at the 400th iteration when  
 172 the cost no longer decreases. The designs recommended by the AM and PSO implementations  
 173 are plotted in Figs. 5 (a) and (b). Even though these two designs yield almost the same level  
 174 of field enhancement, 11.32% and 11.3%, respectively, the designs recommended by these two  
 175 methods have one very distinct difference. The permittivity profile of the AM design is very  
 176 smooth, whereas the PSO design has abrupt changes. The reason behind the smooth design of  
 177 AM is that the permittivity update equation, Eq. (7), is basically an averaging operation that  
 178 includes the contributions of hundreds of interactions between forward and backward fields.  
 179 From a practical point of view, the AM design is easier to fabricate, for example, using thin  
 180 films of acrylonitrile butadiene styrene-based nanocomposites, whose relative permittivity can  
 181 be tuned to any value between 2 and 7 by changing the ferroelectric barium titanate nanoparticle  
 182 fill ratio [31]. As pointed out earlier, PSO-like numerical optimization methods face challenges  
 183 in handling continuous design spaces when the number of parameters to be optimized is large.

184 In terms of computing time and efficiency, let's make the following comparison. In the PSO  
 185 implementation, each trial requires only one calculation of (1). Since we use 2400 swarms  
 186 and 400 iterations, we compute nearly one million LMGFs. For the AM implementation, we  
 187 compute 481 sets of LMGFs (240 forward, 240 backward, and 1 source-to-target), which takes  
 188 47 iterations to converge. So, we compute nearly 23 thousand LMGFs. Due to this significant  
 189 difference between the number of LMGFs computed in the PSO and AM implementations, the



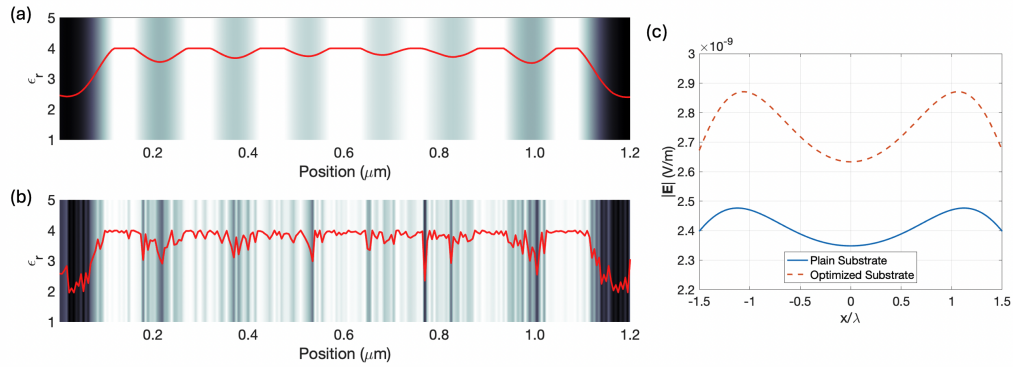


Fig. 5. Permittivity values along the (a) AM and (b) PSO designed substrates with 240 thin layers that lead to an 11.22 % and an 11.2 % enhancement, respectively. (c) Electric field intensity values at  $z = \lambda/2$  and  $-1.5\lambda \leq x \leq 1.5\lambda$ , where  $\lambda = 600$  nm, assuming a plain substrate with relative permittivity of 2 (solid curve) and the optimized substrate (dashed curve).

190 latter requires much less time to achieve the inverse design. We can conclude that the AM not  
 191 only generates realistic designs with smooth permittivity profiles but also achieves the inverse  
 192 design more efficiently than PSO-like numerical optimization algorithms due to calculating the  
 193 gradients based on the laws of physics.

194 It is well known that both the learning rate and dipole sampling density affect the computation  
 195 time and efficiency. For our initial studies, the learning rate was set to 0.01, which provided  
 196 robust but slightly low learning. When we set it to 0.1, we observed oscillations in the cost  
 197 value rather than a continuous and smooth increase. We chose  $\alpha = 0.05$  as the optimum value  
 198 for the examples presented here to balance this trade-off between accuracy and efficiency. In  
 199 short, the learning rate in AM optimization problems determines whether we can achieve our  
 200 goal and, if we can, then how fast we reach our goal. Similarly, when we increase the dipole  
 201 sampling density from  $\lambda/20$  to  $\lambda/30$ , the computation time for each iteration did not change  
 202 due to the recursive calculation of LMGFs. However, we did not observe any reduction in the  
 203 number of iterations during the AM optimization. This verifies that the dipole sampling density  
 204 of  $\lambda/20$  is sufficient to grasp the oscillations in the electromagnetic waves propagating along the  
 205 multi-layered substrate. Using a higher sampling density is neither necessary nor advantageous.  
 206 However, when we reduced the dipole sampling density from  $\lambda/20$  to  $\lambda/10$ , the optimization  
 207 was completed in 161 iterations. The one implemented with  $\lambda/5$  sampling density did not even  
 208 converge. This latter case is probably because a coarser mesh may miss the points where the  
 209 electric field intensity gets maximized, which leads to sub-optimal or inaccurate design solutions.

210 Lastly, we would like to discuss the impact of the observation point range on the efficiency  
 211 and accuracy of the AM implementation. As mentioned before, we calculate the forward and  
 212 backward electric field values over a  $8\lambda$ -wide range horizontally. After including the distance  
 213 between the source and the lower interface of the substrate, we can assume an approximate  
 214 distance of  $5\lambda$  between the source and observation points chosen over the substrate. Again, with  
 215 a rough calculation, this means that both forward and backward electric field intensities near the  
 216 edges of our search domain are one-fifth of the field values calculated along the center, e.g., at  
 217  $x = 0$ . Since the adjoint field calculation includes both terms, the effect over the permittivity  
 218 update of the dipoles near the edges is roughly 4% of those near the center. As a result, their  
 219 contribution is limited to the third digit of the final value of the permittivity for each layer. If one  
 220 is interested in the first two digits only, then a  $3\lambda$ -wide range would suffice.



221 **4.2. Thickness Optimization**

222 In the past two decades, extensive research has focused on monolayers of transition metal  
 223 dichalcogenides, such as molybdenum disulfide ( $\text{MoS}_2$ ) and graphene, commonly called two-  
 224 dimensional (2D) materials. We utilize  $\text{SiO}_2$  coated Si substrates with 90 nm or 270 nm  
 225 thicknesses, illustrated in Fig. 6 (a), to work with these 2D materials. These specific thicknesses  
 226 offer optimal contrast between the coated 2D material and bare regions, facilitating the localization  
 227 of materials during experiments [32]. Our objective is to design a substrate using the adjoint  
 228 method to enhance the visibility of 2D materials further. To achieve this objective, we redefine  
 229 the design question and constraint. Assuming we are limited to two materials,  $\text{SiO}_2$  and Si, but  
 230 have the freedom to choose the number, thickness, and order of layers, we seek the optimal design  
 231 that maximizes contrast for broadband excitation. This optimization problem can be approached  
 232 in various ways. For instance, one might aim to maximize reflectance from the substrate or power  
 233 within the 2D material. We adopt the latter approach.

234 It is essential to note that in this scenario, the source is broadband and far from the substrate,  
 235 similar to the experiments conducted on 2D material-based photodetectors. Due to this large  
 236 distance between the light source and the target, we assume this is a plane-wave-like excitation,  
 237 not a line source. To define broadband excitation, we assume a bell-shaped spectrum ranging  
 238 from 400 to 750 nm, with maximum intensity at 575 nm (normalized to 1) and relative intensities  
 239 of 0.4 at 450 and 700 nm. We assume the monolayer  $\text{MoS}_2$  thickness to be 0.65 nm. The complex  
 240 electrical permittivity of monolayer  $\text{MoS}_2$  is determined using a numerical model accounting for  
 241 the wavelength [33]. Similarly, the electrical permittivity values of Si [34] and  $\text{SiO}_2$  [35] are  
 242 calculated as a function of wavelength.

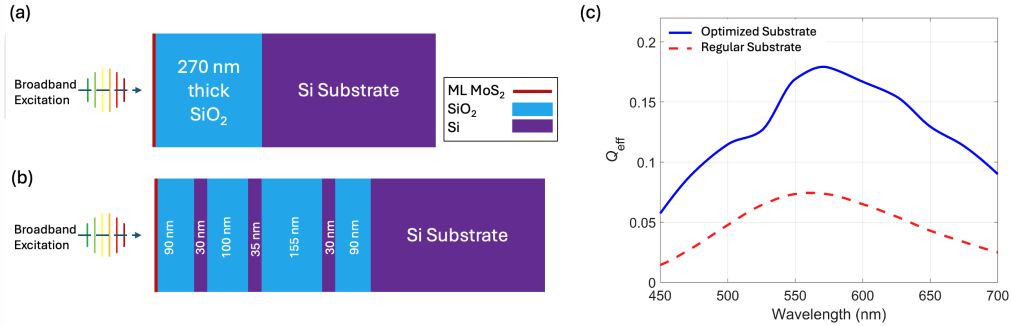


Fig. 6. Monolayer  $\text{MoS}_2$  is placed on top of (a) a simple 270 nm  $\text{SiO}_2$  coated Si substrate, (b) optimized substrate illuminated with a broadband light source, and (c) quantum efficiency of the  $\text{MoS}_2$ -based phototransistors over regular and optimized substrates assuming gate voltage of 10 V, source-to-drain voltage of 0.5 V, and incidence power of  $0.2 \mu\text{W}$ .

243 For the AM optimization, we set the number of inner layers (the layers between  $\text{MoS}_2$  and the  
 244 Si substrate) to 1000, with each inner layer having a thickness of 1 nm. Initially, the material type  
 245 of all the inner layers is set to  $\text{SiO}_2$ . Then, during the iterative process, if the  $\partial\theta/\partial\epsilon_{r,\ell}$  value  
 246 for layer- $\ell$  is larger than the average  $\partial\theta/\partial\epsilon_r$  calculated over all layers, the material of layer- $\ell$   
 247 is set to Si. If the value is lower than the average, then the material of layer- $\ell$  is set to  $\text{SiO}_2$ . The  
 248 inverse design is completed in 88 iterations. The final design, which comprises four pairs of  
 249  $\text{SiO}_2$ /Si layers with different thicknesses, is shown in Fig. 6 (b).

250 To verify the success of the substrate optimization, we first compute the average power ( $E \times H^*$ )  
 251 at the center of the  $\text{MoS}_2$  film using the FDFD solver for both the current industry standard  
 252 substrate shown in Fig. 6 (a) and the one recommended by the AM method as shown in Fig. 6 (b).

253 We achieve to enhance the power absorbed by the MoS<sub>2</sub> film across the entire spectrum, with an  
 254 average enhancement of 72%. Second, we compute the quantum efficiency of the phototransistors  
 255 made from MoS<sub>2</sub> coated SiO<sub>2</sub> substrates as follows.

256 We form a phototransistor by fabricating two metal contacts on opposite sides of a monolayer  
 257 MoS<sub>2</sub> that is placed over a back-gated SiO<sub>2</sub>/Si substrate. This device can convert optical  
 258 excitations into electrical currents, and its quantum efficiency is defined as the ratio of the number  
 259 of generated electrons to the number of incident photons. Briefly, we solve the drift-diffusion  
 260 equations to calculate the output current of the phototransistors numerically [36]. A detailed  
 261 description of how the drift-diffusion model is utilized to compute quantum efficiency and other  
 262 characteristic parameters of 2D material phototransistors can be found in [37]. The quantum  
 263 efficiencies of the phototransistors made with the regular and optimized substrates are shown in  
 264 Fig. 6 (c). It is observed that for the device with a single layer of SiO<sub>2</sub> with a thickness of 270  
 265 nm, the quantum efficiency reaches 7.5% at the wavelength around 561 nm. However, with the  
 266 optimized substrate, the quantum efficiency of 18% is achieved at the wavelength of 571 nm,  
 267 corresponding to a 141 % increase in peak quantum efficiency. The average enhancement across  
 268 the entire spectrum is 210 %.

269 Similar to this example, we can utilize the AM implemented with LMGFs to design a substrate  
 270 that maximizes the field at specific wavelengths while minimizing it at others, accommodating  
 271 different types of excitations, excitation polarizations, and incidence angles. However, implement-  
 272 ing the AM method with a full-wave solver would be necessary for more advanced optimization  
 273 problems, such as if we aim to enhance the fields further based on the surface plasmon resonance  
 274 of metal nanoparticle arrays fabricated on the substrate.

## 275 5. Conclusion

276 This study demonstrates the effectiveness of the adjoint method (AM) combined with layered  
 277 medium Green's functions (LMGFs) for substrate optimization. Through appropriate formulation  
 278 of the optimization problem and constraints, we harness the unique advantages of AM, which  
 279 include efficient computation of gradients and suitability for continuous design spaces, to  
 280 optimize substrate designs aimed at enhancing field properties and transmission characteristics.  
 281 Our numerical investigations illustrate the proposed methodology's accuracy, efficiency, and  
 282 versatility, resulting in significant improvements in field intensity for a selected wavelength or  
 283 wavelength range. Through comparative analysis with particle swarm optimization, we emphasize  
 284 the superior computational efficiency of AM, highlighting its role as a robust tool for photonics  
 285 inverse design.

## 286 6. Appendix

287 The non-zero elements of  $\mathbf{A}$  are as follows,

$$A_{11} = \frac{1}{u_0}, A_{12} = -\frac{e^{-u_1 h_1}}{u_1}, A_{13} = -\frac{1}{u_1}, \quad (9)$$

$$A_{21} = \frac{1}{\epsilon_0}, A_{22} = -\frac{e^{-u_1 h_1}}{\epsilon_1}, A_{23} = \frac{1}{\epsilon_1}, \quad (10)$$

$$A_{21} = \frac{1}{\epsilon_0}, A_{22} = -\frac{e^{-u_1 h_1}}{\epsilon_1}, A_{23} = \frac{1}{\epsilon_1}, \quad (11)$$

$$A_{2N-1,2N-2} = \frac{1}{u_{n-1}}, A_{2N-1,2N} = -\frac{1}{u_n}, A_{2N-1,2N-1} = \frac{e^{-u_{n-1} h_{n-1}}}{u_{n-1}}, \quad (12)$$

$$A_{2N,2N-2} = \frac{1}{\epsilon_{n-1}}, A_{2N,2N} = \frac{1}{\epsilon_n}, A_{2N,2N-1} = -\frac{e^{-u_{n-1} h_{n-1}}}{\epsilon_{n-1}}, \quad (13)$$

292

$$A_{2N,2N-2} = \frac{1}{\epsilon_{n-1}}, A_{2N,2N} = \frac{1}{\epsilon_n}, A_{2N,2N-1} = -\frac{e^{-u_{n-1}h_{n-1}}}{\epsilon_{n-1}}, \quad (14)$$

293

$$A_{2i-1,2i-2} = \frac{1}{u_{i-1}}, A_{2i-1,2i-1} = \frac{e^{-u_{i-1}h_{i-1}}}{u_{i-1}}, \quad (15)$$

$$A_{2i-1,2i} = -\frac{e^{-u_i h_i}}{u_i}, A_{2i-1,2i+1} = -\frac{1}{u_i},$$

294

$$A_{2i,2i-2} = \frac{1}{\epsilon_{i-1}}, A_{2i,2i-1} = -\frac{e^{-u_{i-1}h_{i-1}}}{\epsilon_{i-1}}, \quad (16)$$

$$A_{2i,2i} = -\frac{e^{-u_i h_i}}{\epsilon_i}, A_{2i,2i+1} = \frac{1}{\epsilon_i},$$

295 where  $i = 2, \dots, N - 1$ .296 **References**

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