Broadband Substrate Optimization with Adjoint Method and Green's Functions

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***Abstract*—We present a computationally efficient optimization technique that combines the two-dimensional layered medium Green's functions with the adjoint method to optimize a multi-layered dielectric substrate, achieving maximum field transmission across the visible spectrum.**

***Index Terms*—optimization, multilayered substrate, layered medium Green's function, adjoint method.**

I. Introduction

Figure 1 illustrates a microscope illuminated from below and a simple setup to mimic the light propagation through the substrate in these microscopes. By arranging the thickness and material composition, we can design multi-layered substrates that maximize or minimize transmission or reflection at certain wavelengths for applications in imaging [1] and sensing [2]. We can carry out this substrate engineering using the adjoint method (AM) [3]–[7], which has become quite popular among the inverse photonic design community in the last decade. AM is typically implemented with the finite-differences frequency-domain (FDFD) method [3]–[5] or the transfer matrix method [7]. In this work, we follow a different strategy and implement the AM with layered medium Green's functions (LMGFs). The main advantage of this approach is its computational efficiency compared to the FDFD implementation due to the following important detail: We calculate all the LMGFs at the observation points that are parallel to the interfaces in a single numerical integration. As a case study, we design a multilayered substrate that yields the highest amount of transmission for wavelengths ranging from 400 nm to 700 nm. The FDFD and LMGF implementations produce almost the same substrate. However, despite using the same meshing criteria, the LMGF implementation takes half the time used by the FDFD implementation.

II. Methodology

A. Layered Medium Green's Function

We assume a multilayered medium with $N+1$ layers, where layer-l is defined with thickness h_l and relative electrical permittivity ($\varepsilon_{r,l}$) for $l = 0, 1, \cdots, N$. The interface between the layers l and $l+1$ is parallel to the xy-plane at $z = z_{l+1}$. The wavenumber in layer-l is $k_l^2 = \omega^2 \varepsilon_l \mu_l$, where $\omega = 2\pi f$ and f is the frequency of the electromagnetic waves created by the line source.

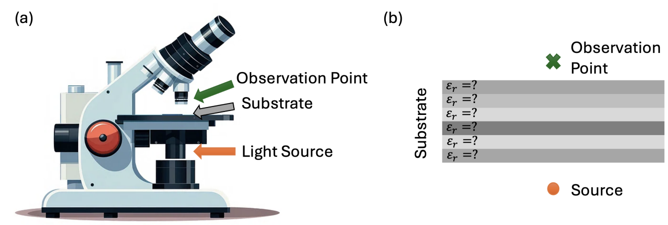

Fig. 1. (a) A microscope illuminated from the bottom and (b) the geometric representation of our problem of interest.

We can obtain the electric field at any observation point (x,z) when the source is located at (x',z') by evaluating the Sommerfeld integral [8],

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

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

$$\tilde{G}(x,z|x',z') = \Phi_l e^{u_l(z-z_l)} + \Psi_l e^{-u_l(z-z_{l-1})}, \quad (2)$$

where k_x is the integration variable, $k_{z,l}^2 + k_x^2 = k_l^2$, and $u_l = jk_{z,l}$. Here, the quantities Φ_l and Ψ_l are unknown. By imposing the boundary conditions for the electric and magnetic fields at the interfaces, we represent Eq. (2) with a linear equation, $\mathbf{AX} = \mathbf{S}$. After calculating the unknown coefficients, we can numerically compute the definite integral in Eq. (1) using a Gauss-Legendre quadrature. However, one should recognize that (i) for the observation points, which are parallel to the xy-plane, it is only necessary to calculate the spectral domain LMGF once, and (ii) numerical integration of this spectral domain LMGF for several observation points sharing the same z can be achieved via a single matrix-vector multiplication. These two facts lead to a reduction by a factor of almost n_x in the computation time compared to the FDFD implementation, where n_x is the number of the cells along the x-axis.

B. Adjoint Method

We will consider here an example in which the goal is to maximize the electric field intensity at a target point located at (x_t, z_t) for n wavelength values. For wavelength-n, the gradient of the cost function (ϑ_n) is

$$\frac{\partial \vartheta_n}{\partial \varepsilon_{r,l}} = -2k_0^2 \sum_d \mathrm{Re}\left\{ E_{l,n}^{\mathrm{forw}} \cdot E_{l,n}^{\mathrm{adj}} \right\} \quad (3)$$

where $E_{l,n}^{\text{forw}}$ is the electric field at the observation point (x,z) when source is located at (x',z') and $E_{l,n}^{\text{adj}}$ is the adjoint field computed using the following expression

$$E_{l,n}^{\text{adj}} = \frac{2j}{\omega_n} E_n^*(x_t,z_t|x',z') E_{l,n}^{\text{back}}(x_d,z_d|x_t,z_t). \tag{4}$$

where $E_n^*(x_t,z_t|x',z')$ is the complex conjugate of the electric field intensity calculated at (x_t,z_t) during the forward calculation, $E_{l,n}^{\text{back}}(x_d,z_d|x_t,z_t)$ is the electric field at the observation point when the source is located at the target point (x_t,z_t). In every optimization step, we update the permittivity using Eq. (3) and the following equation

$$\varepsilon_{r,l}^{\text{new}} = \varepsilon_{r,l}^{\text{current}} + \sum_n \alpha_n \frac{\partial \vartheta_n}{\partial \varepsilon_{r,l}} \tag{5}$$

where α_n is the learning rate. Typically a constant learning rate (α_0) is used. However, in this work, we assume $\alpha_n = w_n \alpha_0$, where w_n is the weight of n-point Gauss–Legendre quadrature, to achieve a uniform broadband enhancement. If the number of iterations reaches a user-defined number or if the permittivity profile stops changing significantly, then the calculations are completed.

III. Numerical Results

As a case study, our goal is to design a 1.2-μm substrate that yields the strongest electric field at at an observation point located 300 nm above the substrate with a point source located 300 nm below the substrate for wavelengths ranging from 400 nm to 700 nm. Additional design constraints are as follows: the minimum layer thickness is 5 nm, and permittivity values cannot be smaller than 2 or larger than 10.

To determine the permittivity profile of the substrate, we assume that the substrate is made from 240 layers, each of which is 5 nm thick. We then implement the AM using both an FDFD solver and LMGFs. For both implementations, we calculate the fields at 800 points along the center of each layer for $-2\ \mu\text{m} \leq x \leq 2\ \mu\text{m}$. At the end of 200 iterations, the FDFD and LMGF implementations produce the permittivity profiles shown in Fig. 2 (a). Although they exhibit strong similarities, the LMGF design is smoother and hence easier to fabricate than the FDFD design. On the same workstation, the LMGF implementation takes 2.5 hours, approximately half the time of the FDFD implementation.

In Fig. 2 (b), we plot the normalized field intensities as a function of incidence wavelength at the observation point for the optimized substrate and two other reference substrates, both of which are 1.2 μm thick but with a constant permittivity of 2 or 10. The normalization is done by dividing the field intensities by the field intensities when no substrate is present. We observe that the optimized design achieves stronger field transmission at all wavelengths. The AM design yields an average field enhancement of 27.3%, while the reference substrates yields enhancements of 9% and 3.9%, respectively.

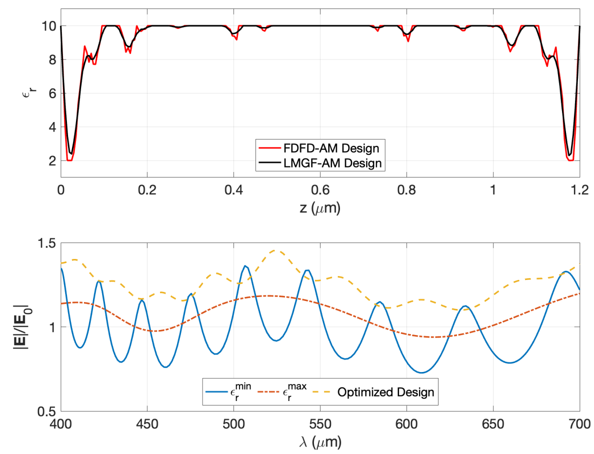

Fig. 2. (a) Permittivity profiles of the AM optimized designs implemented with the FDFD and LMGF solvers. (b) Normalized electric field intensities above two substrates with a permittivity of 2 and 10 and above the substrate with a permittivity profile optimized by LMGF-AF.

IV. Conclusion

We have described a novel computational approach utilizing the layered medium Green's functions (LMGFs) coupled with the adjoint method to efficiently optimize multi-layered dielectric substrates for maximum transmission across the visible spectrum. By exploiting the advantages of LMGF, we were able to reduce computation time by half compared to conventional finite-difference frequency-domain methods. Our method demonstrated its efficacy through a case study, designing a multi-layered substrate yielding significant transmission enhancement over the visible spectrum compared to substrates with constant permittivity.

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