Theory and practical considerations of multilayer dielectric thin-film stacks in Ag-coated hollow waveguides

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This analysis explores the theory and design of dielectric multilayer reflection-enhancing thin film stacks based on high and low refractive index alternating layers of cadmium sulfide (CdS) and lead sulfide (PbS) on silver (Ag)-coated hollow glass waveguides (HGWs) for low loss transmission at midinfrared wavelengths. The fundamentals for determining propagation losses in such multilayer thin-film-coated Ag hollow waveguides is thoroughly discussed, and forms the basis for further theoretical analysis presented in this study. The effects on propagation loss resulting from several key parameters of these multilayer thin film stacks is further explored in order to bridge the gap between results predicted through calculation under ideal conditions and deviations from such ideal models that often arise in practice. In particular, the effects on loss due to the number of dielectric thin film layers deposited, deviation from ideal individual layer thicknesses, and surface roughness related scattering losses are presented and thoroughly investigated. Through such extensive theoretical analysis the level of understanding of the underlying loss mechanisms of multilayer thin-film Ag-coated HGWs is greatly advanced, considerably increasing the potential practical development of next-generation ultralow-loss mid-IR Ag/multilayer dielectric-coated HGWs. © 2013 Optical Society of America

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1. Introduction

Hollow glass waveguides (HGWs) have been widely used in a variety of applications requiring the low-loss transmission of infrared radiation, ranging from high-powered medical laser delivery to broadband spectroscopic chemical gas sensing. In contrast to other current types of infrared waveguides and optical fibers, HGWs have a variety of advantages, including no end reflection, chemical and mechanical stability, high throughput power thresholds, broadband transmission, and easily tunable optical response to meet the requirements of a particular application. HGWs consist of a fused silica capillary, usually of constant bore radius, a, whose inner surface is coated with a uniform reflective silver (Ag) film approximately 200 nm thick, followed by a dielectric thin film of adequate thickness, depending on the desired optical response [1,2]. This dielectric thin-film enhances the reflectivity, thus lowering the propagation loss of the waveguide through constructive interference effects. Commonly deposited dielectric thin film materials in HGWs include silver iodide (AgI), cadmium sulfide (CdS), lead sulfide (PbS), and more recently polymers such as polystyrene (PS) [1,3].

As will be discussed in further detail in the proceeding section, the propagation loss of hollow
waveguides (HWs) depends directly on the waveguide bore size, the angle of propagation of the guided ray, and the reflectance of the inner waveguide surface. Of these loss-determining parameters, both the waveguide bore and the propagation angle are largely fixed by the target application and, as such, cannot be altered to decrease the overall propagation loss. This then leaves the inner surface reflectance as the only practical tunable parameter in reducing HW losses. As previously mentioned, HGWs have traditionally made use of only a single reflection-enhancing dielectric film, yet the use of a single dielectric thin film can only reduce the propagation loss so much, depending on the refractive index of the dielectric thin film material used, the quality of the deposited dielectric and Ag films, and of course the thickness of the dielectric thin film. Even when considering perfect film quality and optimal film thickness, the maximum achievable loss reduction when using a single dielectric thin film is limited and has been calculated to occur when the refractive index of the dielectric material is 1.414. To further reduce propagation losses in HWs in hopes of developing next-generation ultralow-loss HGWs, it is therefore necessary to pursue an increase in waveguide surface reflectance through an alternative method.

Of the limited possibilities in achieving such a desired substantial increase in reflectance, the most obvious and practical is the incorporation of reflection-enhancing low and high refractive index alternating thin film stacks in lieu of a single dielectric thin film, thus having the potential of alternating thin film stacks in lieu of a single reflection-enhancing low and high refractive index material and, as such, the proceeding analysis will consistently incorporate this. Furthermore, the thickness of the innermost (surface) layer must differ from those layers composed of the same material within the multilayer structure and will depend on the total number of layers and whether an odd or even total number of layers are incorporated in the structure, as will be discussed in further detail. By introducing multilayer dielectric stack structures to enhance the reflectivity of HGWs, the reflectance can be considerably increased, particularly as the number of total alternating low and high index layers increases and as the refractive index mismatch of the constituent layer materials increases. Of the commonly deposited dielectric film materials, CdS (\( n_{\text{CdS}} \approx n_L \approx 2.25 \)) and PbS (\( n_{\text{PbS}} \approx n_H \approx 4.25 \)) pose as excellent candidates for the development of such multilayer stacks, due to their high IR transparency, well-developed deposition procedures, chemical compatibility and, above all, their high index mismatch (\( n_{\text{PbS}}/n_{\text{CdS}} = n_H/n_L \approx 1.85 \)). As such, this study will focus exclusively on the use of these two materials in HGWs for the theoretical analysis of said proposed multilayer structures. The proceeding analysis will extend past the point of ideal Ag/multilayer coatings in HGWs to explore the effects of challenges often seen in practice, particularly due to film thickness variability and the introduction of scattering loss due to inevitable surface roughness.

2. Calculation of Waveguide Propagation Losses

Propagation loss in HWs can be theoretically determined via several methods, involving, most commonly, either a wave or ray-optics approach depending on the type of analysis desired. While the wave-optics approach, thoroughly developed by Miyagi and Kawakami, is most suitable for direct determination of propagation losses for specific propagating modes, it inherently assumes that all dielectric thin-film(s) are of optimal thickness for the wavelength of light used in the calculation. As such, this model is most appropriate for determining propagation loss as a function of propagating mode at a specific target wavelength, rather than for determining the broadband spectral response of the waveguide for which the thickness of the individual layer(s) may or may not be optimized depending on the wavelength of light. In contrast, through the ray-optics approach previously analyzed by Miyagi and Matsuura et al., the waveguide loss can be determined as a function of wavelength with freedom in the variability of the thickness of the individual layer(s) in the dielectric waveguide structure. Through this approach, the treatment of propagating light rays at any propagation angle is inherent and, as such, lends itself to much simpler analysis of propagation losses in more unconventional waveguide configurations than the wave-optics approach, such as in waveguides subjected to an applied external curvature and/or tapered bore HWs in which the propagation angle may be dynamic in nature. Most

![Fig. 1. (a) Cross-sectional representation of Ag/multilayer dielectric stack-coated HGW and (b) representative refractive index profile of functional HGW thin films.](image-url)
importantly for the present analysis, however, the ray-optics approach to determining HW attenuation depends directly on the reflectivity of the inner HW surface due to the Ag/multilayer structure and, as such, the reflectivity can be found as a function of the structure in question and then used to determine the waveguide loss.

A. Ray-Optics Calculation of Waveguide Loss

In determining the waveguide loss through ray-optics analysis, the focus will be placed exclusively on meridional light rays propagating along a straight HW of constant bore size. While skew rays may propagate short distances along the waveguide length, their contribution to the total waveguide loss is much smaller than that of meridional rays and can be considered negligible for waveguides of lengths appreciable for any practical applications [1, 4, 13, 14]. In considering a propagating meridional ray along a HW of bore radius $a$, with propagation angle $\phi$ with respect to the optic axis, as presented in Fig. 2, it can be seen that its loss depends on the reflectivity of the inner waveguide surface at each successive reflection. From trigonometric analysis, for a ray of constant propagation angle, the distance between each successive reflection, $L$, is given by Eq. (1) \[ L = \frac{2a}{\tan \phi} = 2a \cot \phi. \] (1)

The length between successive reflections thus depends on the bore size and the propagation angle, increasing with decreasing propagation angle and increasing bore size. The additional ray displacement along the optic axis due to the Goos–Hänchen shift at each reflection is very small relative to the length between each successive reflection has negligible contribution in the calculation and is thus omitted [15, 16]. The number of reflections per unit length is then inversely proportional to this quantity, with the power attenuation coefficient, $2a$, being equal to the number of reflections per unit length times the absorption loss of the inner HW surface structure. This then gives the HW attenuation per unit length in units of dB/m as a function of propagation angle, bore size, and inner surface reflectance as [13, 14]

\[ 2a = 10 \cdot \frac{A}{2a \cot \phi} \rightarrow a = 10 \cdot \frac{1 - R(\phi)}{4a \cot \phi} , \] (2)

where the inner surface reflectance, $R$, is itself a function of propagation angle and several other quantities to be subsequently discussed. Using this ray-optics method for determining the loss of meridional rays in HWs, the modeling versatility for the pursuing analysis of multilayer dielectric thin film stacks in Ag-coated HGWs is inherent and is thus adopted as the foundation for this study.

B. Reflectance Calculation via Transfer Matrix Method

The task then becomes calculating the reflection coefficient of an Ag/multilayer dielectric stack structure as a function of wavelength, layer materials and thicknesses, and incident angle, $\theta = 90 - \phi$. Of the several mathematical methods in determining the reflectivity of such an Ag/multilayer dielectric stack-coated HGW structure, perhaps the most versatile and convenient, and that used in this study, is the transfer matrix method. The transfer matrix method inherently allows for the determination of the reflection coefficient for a multilayer structure with $N$ finite number of thin films by relating the backward and forward propagating field amplitudes across each layer [5, 7, 8]. For an interface, this is achieved with a matching matrix characteristic to the particular interface and, for propagation through each layer, this is achieved with a propagation matrix characteristic to the particular layer material. Eq. (3) defines the characteristic transfer matrix, $[T_i]$, for the propagation of a light ray at an interface between the $i-1$th and $i$th layers and subsequent propagation through the $i$th layer [5],

\[ [T_i] = \frac{1}{\tau_{i-1,i}} \begin{bmatrix} 1 & \rho_{i-1,i} & 0 \\ 0 & 0 & e^{-jk_i d_i} \end{bmatrix} \] (3)

where $k_i$ is the wavenumber of light in the $i$th layer, $d_i$ is the thickness of the $i$th layer, and $\tau_{i-1,i}$ and $\rho_{i-1,1}$, are the transverse Fresnel transmission and reflection coefficients, respectively, between the $i-1$th and $i$th layers, defined for $s$ and $p$ polarized light by Eqs. (5) as follows [5, 8]:

\[ \rho_{si-1,i} = \frac{\eta_i \cos(\theta_i) - \eta_{i-1} \cos(\theta_{i-1})}{\eta_i \cos(\theta_i) + \eta_{i-1} \cos(\theta_{i-1})}, \] (4a)

\[ \tau_{si-1,i} = \frac{2 \eta_i \cos(\theta_i)}{\eta_i \cos(\theta_i) + \eta_{i-1} \cos(\theta_{i-1})}, \] (4b)

\[ \rho_{pi-1,i} = \frac{\eta_i \cos(\theta_i) - \eta_{i-1} \cos(\theta_{i-1})}{\eta_i \cos(\theta_i) + \eta_{i-1} \cos(\theta_{i-1})}, \] (4c)

\[ \tau_{pi-1,i} = \frac{2 \eta_i \cos(\theta_i)}{\eta_i \cos(\theta_i) + \eta_{i-1} \cos(\theta_{i-1})}, \] (4d)
where \( \eta_i \) and \( \eta_{i-1} \) are the impedances of the \( i \)th and \( i \)th – 1 layer materials, respectively. The characteristic matrix for the entire multilayer dielectric film stack, \([T_N]\), is then the product of the characteristic matrices for each interface matching/layer propagation characteristic matrices \([T_i]\) up to \( N \) total number of layers

\[
[T_N] = \prod_{i=1}^{N} [T_i].
\]  
(5)

where it should be noted that the “zeroth” layer is the initial medium of incidence or, in this case, free space. Furthermore, to account for the reflection of the interface between the dielectric layer closest to the Ag film and the Ag film, \([T_N]\) is multiplied by the matching matrix for this interface to yield the characteristic matrix of the entire Ag/multilayer structure system, \([T]\)

\[
[T] = [T_N] \frac{1}{\eta_{N,Ag}} \left[ \begin{array}{cc} 1 & \rho_{N,Ag} \\ \rho_{N,Ag} & 1 \end{array} \right].
\]  
(6)

Considering that the amplitude of the incident light on the system is unity \((E_0^+ = 1)\), and there is no backward propagating wave from the Ag film \((E_{Ag}^- = 0)\), the reflection coefficient of the system is then determined from this characteristic product matrix for the entire system as in Eq. \(9\) [5,8]

\[
\begin{bmatrix} E_0^+ \\ E_0^- \end{bmatrix} = [T] \begin{bmatrix} E_{Ag}^+ \\ E_{Ag}^- \end{bmatrix} \rightarrow \begin{bmatrix} 1/E_0^- \\ E_0^- \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} E_{Ag}^+ \\ 0 \end{bmatrix}.
\]  
(7a)

\[
\begin{cases} \frac{1}{E_0^+} = E_{Ag}^+ T_{11} \\ E_0^- = E_{Ag}^- T_{21} \end{cases} \rightarrow \begin{cases} E_{Ag}^+ = \frac{T_{11}}{T_{21}} \\ E_0^- = \frac{T_{21}}{T_{11}} \end{cases} \rightarrow r = \frac{E_0^-}{E_0^+} = \frac{T_{21}}{T_{11}}.
\]  
(7b)

\[
R = |rr^*| = \left| \left( \frac{T_{21}}{T_{11}} \right) \cdot \left( \frac{T_{21}}{T_{11}} \right)^* \right|.
\]  
(7c)

This calculation is carried out for both \( s \) and \( p \) polarized light in order to obtain the total reflection of the system, and hence the inner surface of the HW. This reflection coefficient is used in conjunction with Eq. \(2\) to determine the propagation loss of an Ag/multilayer-coated HGW having a total of \( N \) reflection-enhancing alternating dielectric thin films. This methodology was used throughout this study to determine the spectral optical loss of the various multilayer structures analyzed in this study. An iterative approach was used in MATLAB to determine attenuation for a given structure as a function of wavelength and angle of propagation.

3. Fundamentals of Reducing Loss via Multilayer Structures

In exploring reflection-enhancing multilayer dielectric thin film stacks, focus will first be placed on the effect of the total number of layers on the overall waveguide loss. For all calculations in this study, with the exception of the forthcoming analysis of waveguide loss as a function of bore size, a constant waveguide bore size of \( a = 350 \mu m \) (ID = 2\( a = 700 \mu m \)) will be assumed, as this bore size is often used for the majority of practical HGW applications. Furthermore, as mentioned in the introduction, the dielectric thin film materials considered will remain constant throughout with CdS being used as the low index material and PbS as the high index material, with the film adjacent to the silver film composed of the low index material (CdS) [1,11]. These dielectric materials will be assumed to be lossless in the \( \lambda = 1–12 \mu m \) region of interest, an assumption which is largely valid except for PbS close to \( \lambda = 1.0 \mu m \). For optimal accuracy in the models presented, the refractive index of the dielectric film materials, as well as the Ag film, will depend on wavelength per the dispersion data for these materials reported by Palik [17]. Finally, any given layer will be assumed to be completely uniform, such that film thickness variation does not vary as a function of position along the waveguide length.

A. Calculating Optimal Film Thicknesses

The individual dielectric thin film thickness will depend on the target wavelength(s), with the optimal thickness for all but the innermost (surface) layer for constructive interference being given by [1,4]

\[
d_f = \frac{\lambda_0}{4\sqrt{n_f^2 - 1}},
\]  
(8)

where \( \lambda_0 \) is the target wavelength of minimal propagation loss and \( n_f \) is the refractive index of the dielectric material constituting that particular layer at \( \lambda_0 \). The optimal film thickness for the innermost layer (CdS) depends on whether the total number of layers, \( N \), amounts to an odd or even number, with Miyagi deriving that for an odd number of layers this thickness should be [4]

\[
\delta_L = \frac{\lambda_0}{2\pi\sqrt{n_L^2 - 1}} \tan^{-1} \left( \frac{n_L}{n_H} \left( \frac{n_L}{n_H} \right)^{\left( \frac{n_L^2}{n_H^2} - 1 \right)} \right),
\]  
(9)

where \( n_L \) is the refractive index of the low index material which composes this innermost layer, and \( n_H \) is the refractive index of the high index material. Conversely, in the case of a total number of even
dielectric layers, the optimal thickness of the innermost film (PbS) should be \[ \delta_H = \frac{\lambda_0}{2\pi n_H^2 - 1} \tan^{-1} \left( \sqrt{\frac{n_L^2 - 1}{n_L (n_H^2 - 1)^{\frac{1}{2}}}} \left( \frac{n_H^2}{n_L^2 - 1} \right)^{\frac{1}{2}} \right), \] (10)

where the innermost layer is composed of the high index material. As previously mentioned, to achieve the largest possible increase in reflection for any given number of layers, the layer adjacent to the Ag film should be composed of the low index material. In exploring the effect of total layers deposited on loss, it will be assumed that all layers are of optimal thickness for the target wavelength and the structure consists of perfectly smooth interfaces.

B. Waveguide Loss as a Function of Total Dielectric Layers

Considering an Ag/multilayer-coated HGW consisting of alternating CdS/PbS layers optimized for \( \lambda_0 = 2.94 \mu m \), yielding \( d_{CdS} = 359 \text{ nm} \) (\( n_{CdS} = 2.28 \)) and \( d_{PbS} = 172 \text{ nm} \) (\( n_{PbS} = 4.39 \)), and guided rays with a propagation angle of \( \theta = 1.0^\circ \). This specific wavelength has been chosen for analysis due to it being the emission wavelength of Er:YAG lasers, which have important applications and for which a limited number of IR fibers and waveguides with varying propagation losses are currently available. Figure 3 gives the calculated spectral response in the near and mid-IR for \( N = 2, 5, 8, \) and 11 alternating CdS/PbS layers with CdS being adjacent to the Ag film. Attenuation has been plotted using a logarithmic scale for optimal analysis of loss as a function of increasing number of multilayer dielectric stack layers at \( \lambda_0 = 2.94 \mu m \). From the spectra presented in Fig. 3, the characteristic shift of thin film interference peaks to longer wavelengths as the number of layers increases is clearly evident. Furthermore, it can be seen that through the incorporation of additional layers of optimal thicknesses for the design wavelength of \( \lambda_0 = 2.94 \mu m \), the waveguide propagation loss drops dramatically as \( N \) increases. As the number of layers increases, the loss centered about the design wavelength continues to drop, yielding the expected photonic bandgap response due to such an ideal 1D multilayered dielectric structure [5,6,8]. Figure 4 gives the maximum achievable loss as a function of total number of dielectric layers for this proposed Ag/multilayer dielectric-coated HGW, obtainable only when all films are of perfect quality and of exactly the optimal thickness for maximum reflection enhancement at the design wavelength of \( \lambda_0 = 2.94 \mu m \). From Fig. 4 it is seen that, with the addition of just 4 PbS/CdS alternating layers, the loss decreases by more than an order of magnitude than that attainable using a single CdS film from \(~0.44 \text{ dB/m} \) to \(~0.037 \text{ dB/m} \). The addition of
work standard for theoretical analysis throughout this most applications and has thus been chosen as the
guided ray will be. The angle of propagation of more efficient the coupling from free space to a
propagation angle, (thus the lower the order of the hybrid
where propagating mode of a specific wavelength is
approximated by Eq. (44). For a HW of given bore size,
the corresponding propagation angle for a given propagating mode of a specific wavelength is
approximated by Eq. (11) [13],
\[
\theta_{nm} = \sin^{-1} \left( \frac{u_{nm} \lambda}{2 \pi a} \right),
\]
where \( u_{nm} \) is the mode parameter of the \( n, m \)
hybrid mode, which is the \( m \)th root of the \((n-1)\)
th order Bessel function [1,4,10]. The lower the propagation angle, (thus the lower the order of the hybrid mode) the lower the propagation loss will be and the more efficient the coupling from free space to a
guided ray will be. The angle of propagation of \( \phi = 1.0^\circ \) corresponds to the lowest order modes and is a
coupling angle commonly achieved in practice for most applications and has thus been chosen as the
standard for theoretical analysis throughout this work [1,13]. However, it is also important to determine attenuation as a function of propagation angle, both since it may deviate depending on various coupling conditions and as it may change as it propagates along the waveguide. While for straight guides, such as is assumed in this study, the propagation angle can be assumed constant, this is not the
case for tapered bore waveguides and waveguides subjected to applied external bending [1,18]. As such, determining loss as a function of propagation angle is important in predicting losses under such conditions. Considering a 700 \( \mu m \) ID Ag/multilayer dielectric-coated HW having a total number of \( N = 2, 5, 8, \) and 11 alternating CdS/PbS layers, each of optimal thickness for \( \lambda = 2.94 \mu m \), attenuation as a function of propagation angle assuming no surface roughness at this design wavelength is presented in Fig. 5.

As expected from previous analysis, the overall loss as a function of total layers decreases as the number of layers increases. Furthermore, as suggested from the previous ray-optics analysis and the preceding discussion, it is seen that propagation losses are indeed lowest for near-grazing incidence (corresponding to lower order modes), and sharply increases as the propagation angle increases for practical angles of propagation seen in HGWs (\( \theta \approx 89.9 \sim 85.0^\circ \)). Past these angles, loss is further seen to increase as a function of propagation angle having an approximately cubic relationship. Importantly, Fig. 5 shows that omnidirectional reflective behavior is not achievable using such an Ag/multi-layer dielectric structure as has been shown for other 1D multilayer dielectric thin film stack systems. This is, furthermore, supported by the fact that despite giving rise to a photonic bandgap, this multi-layer system does not meet the criteria required for omnidirectional reflection derived from band theory [5,6,19].

D. Waveguide Loss as a Function of Bore Size

For complete analysis, a brief discussion on waveguide propagation loss as a function of waveguide bore size has been included. Considering HWs of varying bore sizes of \( 2a = 300, 500, 700, \) and 1000 \( \mu m \), with individual dielectric layer thicknesses optimized as previously for \( \lambda_0 = 2.94 \mu m \) and a propagating ray angle of \( \phi = 1.0^\circ \), the losses for these various bore sizes with increasing number of total dielectric layers is determined. These waveguide bore sizes have been particularly selected for analysis as they represent those most commonly employed in HGWs for use at near and mid-IR

Fig. 4. Theoretical waveguide propagation loss at \( \lambda = 2.94 \mu m \) as a function of total CdS/PbS alternating dielectric layers on an Ag-coated HGW of ID = 700 \( \mu m \) assuming an ideal film structure with each film thickness optimized for this wavelength.

10 more PbS/CdS alternating layers yields an overall drop in attenuation of just over three orders of magnitude in comparison to a single CdS layer from \( \sim 0.44 \, \text{dB/m} \) to \( \sim 9.10 \times 10^{-5} \, \text{dB/m} \). Theoretically, the reflection enhancement due to the addition of even just a couple of high index mismatch alternating dielectric layers is very pronounced and poses a lucrative mechanism for greatly reducing propagation losses in HGWs.

C. Waveguide Loss as a Function of Propagation Angle

In practice, it is important to determine loss as a function of propagation angle, which can indirectly predict the loss for the corresponding mode of propagation. In metal/dielectric-coated HGWs, the lowest loss modes have been theoretically and experimentally shown to be hybrid modes, rather than pure TE or TM modes [4]. For a HW of given bore size, the corresponding propagation angle for a given propagating mode of a specific wavelength is approximated by Eq. (11) [13],

Fig. 5. Theoretical waveguide propagation loss at \( \lambda = 2.94 \mu m \) as a function of propagation angle on an Ag-coated HGW for \( N = 2, 5, 8, \) and 11 total dielectric layers.
wavelengths [1,4,13]. To analyze loss as a function of HGW bore size as the number of multilayer dielectric stack films increases from \( N = 1–15 \), propagation losses at the design wavelength of \( \lambda_0 = 2.94 \mu m \) have been calculated and presented in Fig. 6. From Fig. 6, it can be seen that as expected, loss decreases with increasing bore size. From a ray-optics approach, this is due to the fact that fewer reflections are experienced by a ray propagating along a HW of larger bore size than along one of smaller bore size. Extending briefly to wave-optics analysis, this is indicative of lower propagation loss for a given propagating mode as the waveguide bore increases [1,10]. Furthermore, it is seen that the additional loss reduction due to incorporation of an additional layer is constant regardless of bore size. An extension of this analysis to incorporate a larger number of possible waveguide bore sizes confirms the fundamental \( 1/a^3 \) loss dependency of HWs predicted by Miyagi using wave-optics analysis [1,4].

### 4. Practical Considerations in Determining Propagation Loss

In practice, such dramatic reductions in loss with increasing number of dielectric thin film layers as predicted by theory under ideal conditions (no surface roughness and perfectly optimized individual layer thicknesses) is merely idealistic and realistically unattainable. In practice, two major deviations from the previously presented ideal waveguide loss model pose tremendous challenges in the experimental development of such next-generation ultralow-loss Ag/multilayer dielectric-coated HGWs. The first of these encompasses the deviation of individual layer thicknesses due to experimental fabrication procedures from those optimal layer thicknesses mandated by theory. The second is the inherent surface roughness introduced during thin film deposition, and related surface scattering losses. In this section, the effects of both of these undesirable experimental deviations from the ideal model will first be separately analyzed and then combined to derive a more realistic model for predicting the optical response and propagation losses of experimentally achievable Ag/multilayer dielectric HGWs based on CdS/PbS thin films.

#### A. Effect of Individual Film Thickness Variation

While recently concluded studies [12] have attempted to focus exclusively and in depth on the film growth characteristics of both CdS and PbS thin films in HGWs under different deposition conditions in order to obtain an experimentally consistent model capable of yielding the desired film thickness for a given deposition procedure, some variability in thin film thickness is practically inevitable. Of course, individual film thickness variation from theoretically determined optimal thicknesses for a certain target wavelength will result in alteration of the optical response. The question, then, is not whether inevitable film variation will affect the optical response but, rather, to what degree is such variation tolerable so as to prevent too great of a detrimental effect on the waveguide performance. In the simplest cases of film thickness variation, consistently thicker films than optimal will shift the response to longer wavelengths and result in unintentional optimization of the system for some wavelength \( \lambda > \lambda_0 \), while, conversely, consistently thinner films than optimal will shift the response to shorter wavelengths and result in unintentional optimization of the system for some wavelength \( \lambda < \lambda_0 \). As deduced from currently ongoing experimental trials at the fabrication of Ag/multilayer dielectric HGWs based on CdS/PbS layer stacks, film variation seems to be largely random, yielding neither consistently thinner or thicker films than desired. These trials have shown a film thickness variation of approximately \( \pm 8–12\% \) for CdS and \( \pm 10–15\% \) for PbS [12]. Furthermore, through IR spectroscopic analysis, acceptable results have been suggested, up to a maximum of \( N = 8–9 \) total number of layers, using current fabrication methods.

Even when considering just a total of 8 layers, the possible combinations for accounting for variation in the individual film thicknesses of such a structure is very large and impractical to present. As such, the simulated spectral response for four different individual layer thickness variation ranges have been selected and the resulting spectra given in Fig. 7. The optimal film thicknesses upon which the randomly generated thicknesses accounting for layer thickness variation were those for a target wavelength of \( \lambda_0 = 2.94 \mu m \), using a total of \( N = 8 \) layers and assuming perfectly smooth layer interfaces. For the analysis presented in Fig. 7, random film thicknesses within fixed variation ranges for CdS and PbS layers were generated, with the ranges of random film thickness variation for each of the four simulations in Fig. 7 given in Table 1. As seen in Fig. 7, any deviation in individual film thicknesses from the optimal values will result in an increase in attenuation from the minimal possible attenuation for the dielectric multilayer structure, with increasing loss as the thickness variation increases. The magnitude...
of increase in loss due to film thickness variation is largely dependent on both the magnitude in deviation from the optimal thickness for each layer as well as on the deviation across all layers. However, with the degree of film thickness variation explored in this study, the increased loss from the corresponding ideal system is not nearly as detrimental as that posed by surface roughness scattering, as will be discussed in detail in the following section.

In analyzing the effect of film thickness variation on propagation loss, it must be noted that variation of the innermost layer is of particular importance and has the greatest effect on loss out of any other layer in the multilayer structure. To stress the importance of proper innermost film thickness as determined by Eqs. (9) and (10) for an odd and even number of dielectric layers, respectively, Fig. 8 gives the spectra for optimized and nonoptimized innermost layer thicknesses for \( \lambda = 2.94 \, \mu m \) with \( N = 8 \) CdS/PbS alternating layers on an Ag-coated HGW of ID = 700 \( \mu m \) with film variation ranges of (a) CdS: ± 5–7%, PbS: ± 7–10%, (b) CdS: ± 8–10%, PbS: ± 11–14%, (c) CdS: ± 11–13%, PbS: ± 15–18%, and (d) CdS: ± 14–16%, PbS: ± 19–22% with no film variation spectrum for comparison.

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<th>Fig. 7(a)</th>
<th>Variation Range</th>
<th>CdS</th>
<th>PbS</th>
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<tr>
<td>Variation</td>
<td>± 5–7%</td>
<td>± 7–10%</td>
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Fig. 7. Theoretical waveguide propagation in the near and mid-IR for random individual film variation about optimal film thicknesses for \( \lambda = 2.94 \, \mu m \) with \( N = 8 \) CdS/PbS alternating layers on an Ag-coated HGW of ID = 700 \( \mu m \) with film variation ranges of (a) CdS: ± 5–7%, PbS: ± 7–10%, (b) CdS: ± 8–10%, PbS: ± 11–14%, (c) CdS: ± 11–13%, PbS: ± 15–18%, and (d) CdS: ± 14–16%, PbS: ± 19–22% with no film variation spectrum for comparison.
 occurring at the target wavelength and ensure true optimization of the multilayer dielectric stack in enhancing the reflectance and reducing the loss.

B. Effect of Surface Roughness Scattering

In practice, it is impossible to achieve ideal films void of any surface roughness and, as such, investigating the effect of surface roughness on propagation loss is essential. In the presence of surface roughness, the Fresnel transmission and reflection coefficients between the ith and ith – 1 layers [Eqs. (4a)–(4d)] must be modified to account for scattering losses due to an irregular interface. Matsuura and Harrington [15] have suggested the following modification of these coefficients to account for interface surface roughness:

\[ \rho_{i-1,i} = \rho_{i-1,i} \exp \left( -\frac{1}{2} \left( 2k_0 \cdot \sigma_{i-1,i} \cdot n_i \sin(\gamma_i) \right)^2 \right), \]  
(12a)

\[ \tau_{i-1,i} = \tau_{i-1,i} \exp \left( -\frac{1}{2} \left( k_0 \cdot \sigma_{i-1,i} \cdot (n_i \sin(\gamma_i) - n_{i-1} \sin(\gamma_{i-1})) \right)^2 \right), \]  
(12b)

where \( k_0 \) is the free space wavenumber, \( \sigma_{i-1,i} \) is the RMS surface roughness between the ith and ith – 1 layers, \( n_i \) is the refractive index of the layer material in the ith and ith – 1 layers, respectively, and \( \gamma_i \) is the compliment to the angle of refraction, \( \gamma_i = 90 - \theta_i \) and \( \gamma_{i-1} = 90 - \theta_{i-1} \) in the ith and ith – 1 layers, respectively. These modified Fresnel coefficients are calculated for s and p polarizations and used to proceed with the calculation for the reflectance coefficient [Eqs. (5)–(7)]. It should, furthermore, be noted that surface roughness is a compounding effect, with the ith – 1 layer having a total surface roughness equal to that of the underlying ith layer in addition to any further surface roughness arising from the deposition of the ith layer. Considering this continuously compounding additive effect, the introduction of any surface roughness can quickly have a dramatically detrimental effect on loss, increasing greatly as the total number of deposited layers increases. In practice, it is therefore essential to minimize surface roughness contributed during each subsequent layer deposition procedure.

To examine the magnitude of the detrimental effects of surface roughness on the overall optical response of Ag/multilayer dielectric-coated HGWs in a methodological manner, we consider once more a 700 \( \mu \)m ID Ag/multilayer-coated HGW in which all dielectric layer film thicknesses are optimized for \( \lambda = 2.94 \) \( \mu \)m (average film thicknesses not accounting for variation due to surface roughness). Furthermore, for initial spectral analysis, the total number of dielectric layers will be held constant at \( N = 8 \). In contrast to previous analysis, however, the effects of surface roughness will now be taken into account, where it is assumed that each layer, including the underlying Ag film, contribute an RMS surface roughnesses, \( \sigma_{\text{RMS}} \), of 0, 10, 20, 30, and 40 nm for the various simulations presented. Figure 9 gives the calculated spectral response for individual layer and substrate RMS surface roughnesses of 10, 20, 30, and 40 nm, respectively, with that for \( \sigma_{\text{RMS}} = 0 \) (dotted spectrum), being included in each analysis for direct comparison. The highly detrimental effect of increasing surface roughness, holding all other parameters constant is clearly visible, with an overall increase in loss throughout the entire spectral range covered. Particularly, it can be seen that the loss at the design wavelength quickly increases with increasing surface roughness, surpassing that achievable with only a single CdS dielectric film with \( \sigma_{\text{RMS}} = 0 \) nm (\( \alpha \approx 0.44 \) dB/m) at individual layer surface roughness contributions of \( \sigma_{\text{RMS}} = 30–40 \) nm (\( \alpha \approx 0.32–0.65 \) dB/m) despite the dramatic increase in total number of dielectric layers.

Further analysis focusing on attenuation as a function of both total number of dielectric layers and individual layer RMS surface roughness is given.
in Fig. 10. From Fig. 10, several interesting deductions can be made. For one, for moderate roughness contribution per layer, \( \sigma_{RMS} = 10–20 \text{ nm} \), the loss is greater for an even number of layers \((n)\) than for the preceding number of odd layers \((n - 1)\). This phenomenon is also seen for higher individual layer surface roughness contributions at a low number of total layers. This effect can be attributed to the fact that for an even number of layers the innermost layer material is PbS, rather than CdS for an odd number of layers. Having a considerably higher refractive index mismatch, the effects of surface roughness given by Eq. (12) are considerably more pronounced for the first air/PbS interface than for an air/CdS interface in which the index mismatch is not as dramatic. This suggests that, when considering the practical fabrication of Ag/multilayer-coated HGWs, incorporating an odd number of layers is preferable. Moreover, while loss increases dramatically with increasing surface roughness, the reflection enhancement due to an increasing number of layers is greatly reduced with increasing surface roughness as well. In fact, when considering individual layer roughness of 40 nm, it can be seen that the reduction in loss with increasing number of layers is minimal and, after a certain number of layers, surface roughness related scattering losses completely offset the potential for loss reduction due to increasing the number of layers.

At such high layer surface roughness, the effect of adding even up to 15 total dielectric layers results in a theoretical loss greater than that achievable with just a single CdS layer of low surface roughness \( \sigma_{RMS} = 0–10 \text{ nm} \), denoted by dotted line. Extending this analysis, while not presented in Fig. 10, calculations in which each layer contributed a high surface roughness \( \sigma_{RMS} \approx 60–80 \text{ nm} \), exhibited an initial marginal drop in loss with increasing layers followed by an actual increase in loss relative to a single
dielectric film with the addition of further layers. Finally, it should be noted that unacceptably high individual layer contribution surface roughness values ($\sigma_{RMS} > 90\ nm$) yielded only an increase in attenuation with the addition of any subsequent dielectric layers. Thus, in practice, surface roughness presents a great challenge in achieving the theoretical loss reduction potential of Ag/multilayer dielectric-coated HGWs, with the total number of layers that may be deposited to yield an actual reduction in propagation loss being limited by the individual surface roughness magnitudes achieved via the corresponding thin film deposition procedure and the degree of additive surface roughness with the addition of subsequent films.

C. HGW Model Accounting for Experimental Variations

Following from the preceding analysis a theoretical model accounting for both surface roughness related scattering losses and individual layer film thickness variation for predicting the optical response of experimentally fabricated Ag/multilayer dielectric-coated HGWs based on CdS/PbS multilayer stacks with considerably increased precision has been developed. The development of such a model presents a considerable advancement in bridging the current gap between ideal theoretical models for predicting HGW propagation losses and those achieved in practice experimentally. As an example, consider an Ag/CdS/PbS multilayer-coated 700 μm ID HGW with individual film thicknesses optimized for optimal transmission at the Er:YAG emission wavelength of $\lambda_0 = 2.94\ μm$. Furthermore, let us assume individual RMS surface roughness contributions of $\sigma_{RMS} = 15, 25, \ and \ 20\ nm$ for Ag, CdS, and PbS thin-films, respectively, with randomized dielectric film thickness variations of up to approximately ±12% for CdS and ±15% for PbS. Such surface roughness and dielectric film thickness variations from optimal are based upon those frequently seen in previous and ongoing studies in experimental Ag/multilayer-coated HGWs. As for the majority of previous analysis, a propagation angle of $\varphi = 1.0°$ is assumed. Figure 11(a) gives the theoretical propagation loss for such an improved model as a function of total number of dielectric layers. From Fig. 11(a), the greatly diminished propagation loss enhancement for this modified model, in contrast to that predicted by the ideal model, is clearly evident. Using the practical thin-film parameters outlined above, it can be seen that, in practice, the incorporation of additional dielectric layers has a much more marginal effect than that predicted by the ideal model. In particular, it is seen that the addition of a greater number of layers (beyond $N \approx 11$) has very little, if any, additional benefit according to this practical model. Incorporation of multilayer dielectric stacks does reduce the loss compared to incorporating a single dielectric layer below $N = 7$; however, this loss reduction is orders of magnitudes less than ideal. Furthermore, for the incorporation of only a few dielectric layers (below $N \approx 8$), the loss is only reduced from that achieved with a single dielectric layer when there is an odd number of layers in the structure. This phenomenon reflects the discussion presented in the surface roughness related scattering section. As predicted by this practical model, using the aforementioned layer parameters, optimal loss reduction thus occurs around $N = 7$, a number of layers that has been successfully achieved in CdS/PbS multilayer-coated Ag HGWs in ongoing studies. To further stress the combined effects of surface roughness and film variation, Fig 11(b) gives the calculated spectral response for $N = 7$ derived for the practical (modified) model with the given nonideal individual layer parameters along with that predicted by the ideal model (dotted spectrum). Of course, the response calculated using the practical model derived in this analysis will depend strongly on surface roughness for the individual films in the reflection-enhancing structure as well as the film variation of the dielectric layers from optimal thicknesses and, as such, lends itself to modification according to such values achievable by the particular deposition procedure.

Fig. 11. (a) Calculated waveguide loss at $\lambda = 2.94\ μm$ as a function of total CdS/PbS alternating dielectric layers on an Ag-coated HGW according to the modified propagation loss model and (b) calculated spectral response of an Ag/multilayer-coated HGW with $N = 7$ according to this modified model along with that for the ideal model for comparison.
5. Conclusion
In this study, a theoretical model for predicting the optical response, in particular the propagation loss of HGWs, incorporating any number of reflection-enhancing dielectric thin-film(s) is presented. This model, based on ray-optics analysis, lends itself to great versatility, in particular relative to those previously presented in the literature, mostly due to the incorporation of the highly flexible transfer matrix method for determining the reflectance of the particular Ag/single or multilayer dielectric inner HGW surface structure. In particular, the transfer matrix method is highly advantageous relative to other methods for calculating this reflectance, due to its inherent ability to calculate wavelength dependent reflectance of the structure for any number of dielectric layers while simultaneously accounting for deviations in the individual structure layers from ideal, such as individual film variation and surface roughness, without appreciable modification of the simulation algorithm other than the specific layer parameters. As such, analysis of Ag/multilayer-coated HGWs based on practical CdS/PbS alternating layer thin film structures is extended well beyond the ideal model and the effects of increasing surface roughness and individual thin film thickness variation as a function of increasing the number of total CdS/PbS alternating layers is thoroughly examined. Such analysis is then combined to derive a much more precise practical model for determining propagation losses in Ag/multilayer-coated HGWs, consequently achieving a theoretical model which much more closely approaches experimentally achieved propagation losses. While this model is not a perfect match to experimentally achieved losses as it cannot accurately account for further experimental error and random imperfections and assumes complete transparency of CdS and PbS thin films across the near and mid-IR $\lambda = 1–12 \, \mu m$ region, it provides a much more advanced, practical, and accurate model for predicting propagation loss in HGWs and, as such, provides a much more invaluable tool for the engineering and design of Ag/multilayer-coated HGWs relative to widely used idealistic models.

Through such a practical model, the effects of individual layer surface roughness and thickness variation from optimal values on HGW propagation losses has been thoroughly analyzed and compared to those predicted by theory not accounting for these practical considerations. In particular, the importance of achieving adequate individual layer film thicknesses has been investigated, with analysis showing that achieving an adequate innermost film thickness depending on the total number of structure layers has a highly pronounced effect on the achievable propagation loss for the desired target wavelength. Furthermore, extensive analysis of the effect of film surface roughness on loss concludes that increased surface roughness has a much more pronounced detrimental effect on loss than film thickness variation. In particular, it was shown that even a relatively small increase in individual layer surface roughness greatly reduces the reflection-enhancing effects of incorporating an additional number of CdS/PbS alternating layers. This effect is so detrimental in fact that, given a high enough surface roughness of the individual layers in the structure, the benefit of incorporating additional layers decreases significantly with increasing surface roughness, even yielding an increase in loss with increasing total number of layers. In practice, the particular optical response will depend on a number of experiment specific achievable parameters, most notably the total number of layers in the structure, the individual layer variation from optimal for a given target wavelength, and the individual layer surface roughness contribution and, as such, these must be modified accordingly in the practical model derived in this study. Most notably, given typical experimental parameter values achieved using current deposition procedures, it has been shown that the incorporation of additional CdS/PbS alternating layers for maximum transmission at $\lambda_0 = 2.94 \, \mu m$ is only beneficial up to a certain number of total layers, after which this becomes only marginally advantageous and does not offset the risks posed by the deposition of subsequent layers through current experimental procedures.

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