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Design of Palladium Coated Long Period Fiber Grating for Hydrogen Sensing

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Abstract—We present a detailed numerical analysis that describes the influence of palladium (Pd) layer thickness on the spectral characteristics of long period fiber gratings (LPFGs) and their response to the uptake of hydrogen. The investigation is carried out with a view of determining an optimal layer thickness to design high sensitivity LPFG based hydrogen sensors. Coupled differential equations for a four layer waveguide structure have been solved using matrix method considering a layer of Pd with finite thickness on the cladding. Response of higher order cladding modes of the Pd-coated LPFG at turn-around-point (TAP) and also at mode transition could be computed. It has been shown that if properly designed, the resonant wavelength of a desired mode may shift by about 20 nm for 1% uptake of hydrogen. There is good match between simulations and experiments for LPFGs with coupling to higher order cladding modes.

Index Terms—Long period fiber gratings, turn-around-point grating, mode transition, palladium coatings, hydrogen detection.

I. INTRODUCTION

Accurate and fast measurement of hydrogen gas concentration and leak detection is essential to prevent the risk of an explosion. Palladium (Pd) coated fiber optic sensors have always been competitive and remain to be a preferred mechanism for hydrogen sensing because of their inherent safety for use in a potentially explosive environment. Extensive summaries of research work are available in the review articles [1-4]. Among several different configurations, Pd coated fiber Bragg gratings (FBGs) and long period fiber gratings (LPFGs) for hydrogen sensing have received special attention. The response of these fiber grating sensors is wavelength encoded which is more reliable and accurate as compared to intensity based measurements and they also offer quasi-distributed sensing characteristics. Even though different Pd coated grating based sensing configurations have been established, there are continuing efforts to improve upon their sensitivity, response time and the reliability. To enhance the sensitivity the use of newer high sensitivity FBGs [5] and several tailor-made Pd alloys and composites [6-8] have been suggested. The stability of these hydrogen sensitive layers has also been studied quite extensively and can be improved by deposition of intermediate layers [1,6]. Apart from sensitivity and stability, the response and recovery time of the sensor is also an important parameter. From the literature review it is utterly clear that the response time of optical sensors, apart from a few configurations, has to be brought down quite dramatically to make them competitive with other technologies available commercially [9]. It has been observed [4] that to get a fast (response time < 10 s) optical fiber hydrogen sensor, a thinner layer (roughly around 10-15 nm or less) of Pd or its alloy is preferable. FBG sensors with thin sensitive films have been tried. In FBG sensors, where strain measurement due to volumetric expansion of the Pd layer upon hydrogen intake is a prime requirement [2], thinning the layer certainly would have an adverse effect on the sensitivity. However, the sensitivity of FBGs can be enhanced either through removal of the cladding around the FBG region, by etching, or by using specialty microfiber FBGs.

In these circumstances LPFG sensors can be more useful. The reasons are as follows. Pd coated LPFG sensors are inherently much more sensitive than FBGs in hydrogen sensing [10-12]. The sensitivity can even be enhanced further if higher order modes are selected [13,14]. Secondly, shifts of the resonant wavelengths of a Pd coated LPFG sensor are not solely due to the strain induced by Pd layer but also due to the change in complex refractive index (RI) of the Pd film upon hydrogen uptake [2]. However if the layer thickness is small enough we can neglect the effect of strain on the wavelength shift and the sensor can be modelled considering the effect of RI change of the Pd layer only. With a well designed LPFG sensor it is possible to detect the change in complex RI of the Pd even if it is in the α-phase where the increase in the lattice parameter or the hydrogen adsorption induced strain on the fiber is small. Moreover, when measurement of RI change is the only requirement an ultrathin film should serve the purpose and the response and recovery of the sensor should be fast.

However, though the work on LPFG based hydrogen sensors reported earlier show promising results, the choice of layer thicknesses were somewhat arbitrary. It becomes difficult to obtain a clear idea about the choice of Pd layer thickness for optimum sensitivity from the available literature. Therefore, to have an explicit theoretical data that describes the response of LPFG modes to hydrogen adsorption for varying Pd thickness seems to be the need of the hour. In their previous work [15,16], the authors had modeled a Pd coated LPFG where the Pd layer was considered to be sufficiently thick to act as an infinite layer for the propagating cladding modes. Coupled mode analysis was therefore done for a three layer fiber cross-section, i.e. core-clad and then a layer of infinite Pd based on the methodology as suggested by Erdogan [17]. However, when the LPFG is coated with a thin layer of
Pd, such that the evanescent fields of the propagating cladding modes extend into the environment, then the assumption may not hold good and therefore, coupled mode analysis for a four layer waveguide i.e. core-clad-Pd-air is necessary to investigate the response of LPFG modes to hydrogen uptake.

In this paper we have modeled the transmission spectra for LPFGs coated with thin Pd layers. With detailed numerical simulation it is shown that the effective indices of the cladding modes and in turn the response of the same to hydrogen uptake do change with the thickness of the Pd layer. This implies that the three layer model cannot correctly interpret the shift of the resonance wavelength for a thin Pd layer. We developed the model using the transfer matrix formulation proposed earlier for multilayer dielectric waveguide structure [18].

It should be noted that the theoretical estimation of the spectral shift of Pd coated LPFG modes due to adsorption of hydrogen is a two-step process. In the first step we modeled LPFG spectra with varying Pd thickness. Then in the second step we estimated the shift of resonant modes as a function of the expected changes in the complex RI of Pd following an uptake of hydrogen into the lattice. The modeling becomes a bit tricky in the second step. This is because the effect of low concentrations of hydrogen, on the complex RI of Pd, especially for thin layers, is not very well characterized and some contradicting results are presented in the literature [19-24]. We simulated a range of fractional changes in the complex RI by varying the real and imaginary part independently and in combination over a range of +/- 10% change of the Pd RI when there is no hydrogen in the Pd lattice. The contribution of the changes in the imaginary part of the Pd RI towards the LPFG wavelength shift was found to be quite significant. Our results are able to allow us to exclude some of the previously reported trends in the change of the RI, especially the imaginary part. We validated our assumption by comparing the simulated results with the experiments reported earlier [14]. We extended our investigation to compute the response of higher order modes of a Pd coated LPFG at turn-around-point (TAP) and could show that if properly designed, the sensitivity to hydrogen can be significantly enhanced using a thin Pd layer. Finally, we could establish that with a specific Pd thickness a particular LPFG mode can be operated at its resonant wavelength for hydrogen uptake. This thus proposed design will help the scientific community in the field to design highly sensitive and fast Pd coated LPFG sensors for hydrogen detection.

II. MODELING METHODOLOGY

The generalized transfer matrix formulation based on LP modes for a multilayer dielectric waveguide structure given in [18] is utilized for modeling Pd coated LPFGs. The model consists of a four layer fiber waveguide structure as shown in Fig. 1. The refractive indices of the fiber core, fiber cladding, Pd coating and surrounding air are denoted as $n_1$, $n_2$, $n_3$ and $n_4$, respectively. It is assumed that the core mode (LP$_{0,v}$) couples with only the axially symmetric cladding modes denoted as LP$_{0,v}$, $v > 1$.

Fig. 1. Four layer structure for modeling Pd coated LPFG (not to scale).

The radial field for the cladding mode LP$_{0,v}$ in the $i$th layer is given as [18]

$$E_{0,v,i} = A_{0,v,i} + B_{0,v,i}r \gamma_{0,v,i} + C_{0,v,i}r^{\nu} \gamma_{0,v,i} \nu$$

$$\gamma_{0,v,i} = \frac{k_i^2 n_i^2 - \beta_{0,v}^2}{\beta_{0,v}^2}$$

where, $A_{0,v,i}$ and $B_{0,v,i}$ are arbitrary field expansion coefficients for the $i$th layer.

The characteristic equation is formed as detailed in [18]. The roots of this equation are the propagation constants $\beta_{0,v}$ for the mode LP$_{0,v}$. As the refractive index for the Pd, $n_3$ is complex, the characteristic equations are complex and a zero finding algorithm for complex roots based on Newton’s method is used. The radial fields for the core mode and the cladding modes in each layer have been calculated by substituting the value of $\beta_{0,v}$ in Eqn. (1-2).

The coupling constants for the interaction of the core mode with each of the cladding modes for a longitudinal sinusoidal refractive index modulation in the core were computed as given in [26] and may be represented as

$$\kappa_{01-0v} = \frac{\pi}{\lambda} \Delta n l$$

where $\Delta n$ is the induced index change, $\lambda$ is the overlap integral and $l$ is given by:

$$l = \int_0^{\infty} \frac{E_{co}^2 + E_{c1}^2 - E_{cl}^2}{2} r dr d\phi$$

where $E_{co}$ is the radial field for the core mode, $E_{c1}$ and $E_{cl}$ are the radial fields for the cladding modes LP$_{0,v}$ and $r$ is the radial vector.

The transmission loss has been computed using standard coupled mode equations [17] for LPFG which may be represented as

$$\frac{dA_{01}}{dz} = j\kappa_{01-0v} A_{co} + j\frac{m}{2} \kappa_{01-0v} A_{v} \exp(-j2\delta_{01-0v}z)$$

$$\nu \frac{dA_{0v}}{dz} = j\frac{m}{2} \kappa_{01-0v} A_{co} \exp j2\delta_{01-0v}z$$

where $A_{co}$ and $A_{v}$ are the amplitudes of the core mode and the cladding modes, respectively, $\kappa_{01-0v}$ is the coupling constant for the core-cladding interaction, $\kappa_{01-0v}$ is the coupling constant for the core-cladding interaction, $\kappa_{01-0v}$ is the detuning factor for the core-cladding interaction, $\delta_{01-0v}$ is given by:
\[ \delta_{01-0v} = \frac{1}{2} \beta_{01} - \beta_{0v} - \frac{2\pi}{\Lambda} \]  

(7)

where \( \beta_{01} \) and \( \beta_{0v} \) are the propagation constants for the core and the cladding modes, respectively and \( \Lambda \) is the period of the grating.

The set of ordinary differential equations in (5) and (6) have been represented in matrix form as in [27], assuming \( k_{01,01}^1 = 0 \). These equations are solved numerically using the initial boundary conditions. The square of the amplitude of the core mode at the end of the grating gives the transmitted power.

\[ T = A_{co}(L)^2 \]  

(8)

where \( L \) is the length of the grating.

III. Simulation Results

In this section we present detailed simulation results that deal with computation of spectra of Pd coated LPFG modes and their response to hydrogen. We have estimated the response of cladding modes of different orders which are then corroborated with experimental data. Subsequently, we present the characteristic response of a cladding mode at turn-around-point for a varying thickness of Pd. We also show that with a predesigned layer of Pd, a cladding mode can be taken to its mode transition point where the sensitivity of the mode to hydrogen adsorption becomes significantly high.

A. Parameters Used

In our simulation we consider an SMF28e fiber with core radius = 4.1 \( \mu \)m and cladding radius = 62.5 \( \mu \)m. For our use we computed the core and cladding refractive indices at each wavelength of our interest using coefficients as per the relation given in (12). The Sellmeier coefficients were experimentally derived as reported in previous work by the authors [15,16].

\[ n^2 = 1 + \frac{3 \Lambda_0 \lambda^2}{2 \lambda^2 - B_i} \]  

(12)

This provides a core RI of 1.4494 @ 1550 nm and cladding RI of 1.444 @ 1550 nm. We conducted our initial experiments with LPFGs having a Pd layer of about 60 nm. Therefore, the Sellmeier coefficients of a 60 nm thick Pd layer were used for modeling the spectrum of the Pd coated LPFG. It is important to note that there is a significant level of uncertainty in the exact values for the complex RI of Pd. Literature values vary widely between 3.2 - 3.7 and 8 - 8.5 for the real and imaginary part, respectively [19, 28-30]. Furthermore, it has been reported [31] that the exact values depend on the particular coating technique which has been used. The values used in this paper have been derived experimentally by variable angle ellipsometry and SPR and the coating techniques and parameters used to create the layers for determination of the RI were also used to deposit the coatings on the LPFGs [31]. This provides a complex RI for the Pd layer @ 1550 nm of \( \sim 3.605 + i 8.498 \). The variations of the real and imaginary parts of the Pd RI with wavelength are given in Fig.2(a).

Both real and imaginary parts of the Pd RI vary considerably with film thickness [19], especially for thicknesses where the film is partially transparent with the imaginary part tending towards ‘zero’ and the real part tending towards ‘1’ for a film thickness tending towards ‘zero’. Fig. 2(b) shows a plot of real (‘n’) and imaginary (‘k’) parts of Pd RI versus thickness taken from [19] for a wavelength of 1550 nm and an exponential fit to the data.

The drop in the values of \( n \) and \( k \) at larger thicknesses is an indication of the experimental uncertainties in the determination of these values since it is expected that the actual values should trend towards an asymptotic limit as shown by the fitted line. For obtaining the Pd RI for thin films with varying thickness at each wavelength, the experimentally derived Sellmeier coefficients of a 60 nm Pd film were rescaled for thin Pd films using the values of Pd RI (@ 1550 nm) vs thickness given in fig. 2(b).

Upon adsorption of hydrogen, the RI of the Pd layer changes, leading to changes in the LPFG resonance bands. There are varying reports about the percentage change in the RI of the Pd layer in response to hydrogen [19-24]. It is known that both real and imaginary parts of the permittivity of the Pd films decrease with the adsorption of hydrogen. The real and imaginary parts of the RI (\( n \) and \( k \)) as a function of the real and imaginary parts of the permittivity (\( \varepsilon_1 \) and \( \varepsilon_2 \)) are given as:

\[ n = \frac{\varepsilon_1 + \varepsilon_2 + \varepsilon_5}{2} \]  

\[ k = \frac{\varepsilon_1 + \varepsilon_2 - \varepsilon_5}{2} \]  

Thus, if \( \varepsilon_1 \) and \( \varepsilon_2 \) decrease, \( n \) will also decrease and \( k \) may increase or decrease depending on the value of the permittivity. Thus the real part of the Pd RI will decrease on hydrogen adsorption. As stated earlier, there are considerable variations across literature [19-24], leading to a large uncertainty in the scale and even the sign of the fractional change of the complex RI. However, it is widely accepted that the real part of the RI decreases with increasing hydrogen uptake into the Pd lattice. It is also widely stated that, \( k \), the imaginary part of the RI is more strongly affected by the hydrogen uptake, however, in some literature this change is stated to be positive [19] and in some literature it is stated to be negative [23, 24].

B. Simulation of resonant modes of Pd coated LPFG and validation of data with experiments

A 24 nm long LPFG with 400 \( \mu \)m period, was fabricated using an UV laser by point by point writing technique. The experimentally observed spectrum for the above LPFG is shown by the black solid line in Fig.3. The simulated spectrum, which was computed using the matrix method described in Section II, assuming \( \Delta n = 0.00032 \), is shown by the red dashed line in the same figure. There is a very close match between the two spectra in Fig.3. In the next step, a 60 nm thick Pd coating was deposited on the aforementioned
LPFG by the RF Sputtering technique. A distinct red shift of the resonance wavelength of LP\(_{0.6}\) mode was observed. The resonant wavelength of the other resonant modes from LP\(_{0.5}\) to LP\(_{0.3}\) also had some shift due to deposition of Pd but gradually becomes insignificant as we move towards lower orders. Fig. 4 shows the measured and the simulated spectra of LP\(_{0.2}\) to LP\(_{0.6}\) resonant modes for the above Pd coated LPFG.

![Fig. 3](image)

**Fig. 3.** Spectra for uncoated LPFG on SMF28e with 400 \(\mu\)m period: black solid - experimental, red dashes - simulated.

LPFGs coated with a thin film of Pd have been reported widely and the observed loss bands always exhibit a blue shift for an increase of hydrogen (H\(_2\)) concentration in the Pd lattice. In [32] we report a shift of about -64 pm of the LP\(_{0.6}\) mode in response to an exposure of 1% H\(_2\) at 70ºC for an LPFG coated with a 60nm thick Pd layer. At room temperature, we would have expected a shift of \(-120\) pm due to a change in solubility of hydrogen in Pd [33]. The details of the experimental procedure are available in [32] and will also be included in a paper to be communicated soon. Now to compute this wavelength shift due to adsorption of hydrogen it is necessary to have a reliable data set that describes the change of real and imaginary part of the complex RI of Pd upon hydrogen uptake for different layer thickness, at different temperature and also at different partial pressure. We have already mentioned earlier that in this regard the available data in the literature are not adequate and to some extent conflicting. Therefore, in our simulation we relied on a realistic approach; to assume the percentage change in the real and imaginary part of the Pd layer RI that validates our experimental results. Using our four layer model we computed the wavelength shifts of the LPFG modes for a range of fractional changes in the complex RI by varying the real and imaginary part independently and in combination over a range covering +/− 10% change of the Pd RI when there is no hydrogen in the Pd lattice. For a better understanding, in this simulation we investigated the wavelength shifts of LP\(_{0.6}\), LP\(_{0.9}\) and LP\(_{0.10}\) cladding modes. Computed wavelength shifts for the LP\(_{0.6}\) mode are shown in Fig. 5, where the calculated shift is shown on the z axis and the x and y axes are the fractional changes in the real and imaginary part of the complex RI respectively.

![Fig. 4](image)

**Fig. 4.** Spectra for LPFG on SMF28e coated with 60nm Pd layer with 400 \(\mu\)m period: black solid - experimental, red dashes - simulated.

The lines across the surface indicate all of the possible combinations of fractional changes in \(n\) and \(k\) which would result in a wavelength shift of \(-64\) pm and \(-120\) pm. These lines clearly indicate that all possible solutions only lie in the range of a positive change of the imaginary part, and both positive and negative changes in the real part would be permitted as per this simulation. However, the positive region of the real part is clearly excluded from first principle since an uptake of hydrogen will lead to a strain in the lattice, a reduction in electron mobility and therefore an increase in resistivity, which in turn, via the Drude-Lorentz model, will lead to a decrease in RI.

Our analysis shows that within permissible combinations, the consequence of the % change of the imaginary part of the Pd RI on the shift of resonant wavelength is more predominant as compared to the % change of the real part. Alternatively, we may say that the imaginary part affects the effective index of the cladding mode more than a change in the real part. It has been observed that an increase of 1% in the imaginary part of the Pd RI induces a blue shift of the resonant wavelength by \(-15\) pm and vice versa. On the other hand, an increase of the real part by similar % induces a blue shift of \(-2\) pm and vice versa. Although the exact % change in real and imaginary parts of Pd RI upon exposure to H\(_2\) cannot be inferred from fig. 5, we have obtained a set of combinations of % change in real and imaginary parts of Pd RI, which would lead to -64 pm wavelength shift of the LP\(_{0.6}\) mode of an LPFG coated with a 60 nm thick Pd layer, which in turn corresponds to a 1% H\(_2\) uptake at 70ºC. Thus if we consider any one combination of % change in real and imaginary parts of Pd RI amongst the allowable solutions depicted by the red straight line in Fig. 5.

![Fig. 5](image)

**Fig. 5.** Computed wavelength shifts of LP\(_{0.6}\) loss band of the LPFG coated with a 60 nm thick Pd layer for different % changes in real (n) and imaginary (k) parts of Pd refractive index. The two lines show the possible combinations of fractional changes in \(n\) and \(k\) which would result in a wavelength shift of -64 pm and -120 pm.
for the numerical analysis, we would obtain the same wavelength shift for a particular mode. This is because the composite effect of these different combinations of the real and imaginary components on the effective index of the Pd layer will remain same. For example, if we select three combinations (-1, 4.4), (-5, 5) and (-9, 5.6) from the possible set of solutions on the red straight line in Fig. 5, each of the combinations will have same composite effect on the effective index of the cladding mode and hence result in the same wavelength shift. For our simulations we have chosen the combination of -5% change in real part and 5% change in the imaginary part of Pd RI, which is one of the combinations for an LP_{0.6} wavelength shift of -64 pm and is equivalent to a 1% H\textsubscript{2} uptake at 70°C.

The simulated wavelength shift of the LP_{0.6} resonant loss band for the Pd coated LPFG in presence of 1% H\textsubscript{2}, assuming a -5% change in real part and 5% change in the imaginary part of Pd RI is depicted in Fig.6(a). The same wavelength shift would result for a range of values represented by the red straight line in Fig.5. The LP_{0.6} loss band shifts by ~-64 pm in presence of 1% H\textsubscript{2}. The experimental result for the shift in LP_{0.6} resonant wavelength in presence of 1% H\textsubscript{2} at 70°C is given in Fig.6(b). The result in Fig. 6(b) is the wavelength shift of the LP_{0.6} mode for on and off cycles of 1% H\textsubscript{2} obtained by tracking the peaks in the spectra, showing a shift of ~-64 pm in presence of H\textsubscript{2}.

Higher sensitivities can be achieved for higher order modes. We had fabricated two LPFGs with periods of 237 μm and 213 μm respectively to position the LP_{0.9} and LP_{0.10} resonant modes around 1550 nm. The experimental values of the wavelength shifts in presence of 1% H\textsubscript{2} at 70°C were found to be ~-112 pm and ~-447 pm for the LP_{0.9} and LP_{0.10} modes respectively [14].

Fig. 6. (a) Simulated LP_{0.6} resonant loss bands for the LPFG coated with a 60 nm thick Pd layer, in absence of H\textsubscript{2} (black solid) and in presence of 1% H\textsubscript{2} (red dashes) assuming a -5% change in real part and 5% change in imaginary part, although the same shift is calculated for a range of values shown in Fig.5 and (b) Experimental shift of LP_{0.6} resonant wavelength in presence of 1% H\textsubscript{2}.

Fig. 7. (a) Simulated LP_{0.9} resonant loss bands for the LPFG coated with a 60 nm thick Pd layer, in absence of H\textsubscript{2} (black solid) and in presence of 1% H\textsubscript{2} (red dashes), (b) Experimental shift of LP_{0.9} resonant wavelength in presence of 1% H\textsubscript{2} at 70°C.

The simulated resonant loss bands of the LP_{0.9} and LP_{0.10} modes both in absence of H\textsubscript{2} and in 1% H\textsubscript{2} are shown in Fig.7(a) and Fig.8(a) and the measured values for the respective cases are shown in Fig.7(b) and Fig.8(b).

The simulated wavelength shifts in presence of 1% H\textsubscript{2} are -130 pm and -400 pm for the LP_{0.9} and LP_{0.10} modes, respectively and are found to have an excellent match with the measured value. In this simulation we considered a -5% change in real part and 5% change in imaginary part of the RI of Pd which justifies the consistency of our assumption as derived from the previous experiment.

C. Response of cladding modes to Pd thickness around mode transition

In this section we present the influence of Pd layer thickness on the sensitivity of cladding modes in more detail. We compute the variation of the effective indices of first eleven cladding modes i.e. LP_{0.2-12} as a function of Pd layer thickness. The result is shown in Fig 9. We have considered the change in n and k as a function of Pd layer thickness into account in our simulation. It may be seen that the effective indices of the clad modes increase with Pd layer thickness and in the region of Pd layer thickness from 10 to 16 nm a rapid change in n\textsubscript{eff} is observed as reported earlier for the case of a high refractive index dielectric overlay on LPFG [25]. This corresponds to the transition region in which we expect the LPFG to have significantly high sensitivity towards even small changes in the RI of the Pd layer which affect n\textsubscript{eff} of the cladding modes and thereby the loss band position of the associated modes.

Fig. 8. (a) Simulated LP_{0.10} resonant loss bands for the LPFG coated with a 60 nm thick Pd layer, in absence of H\textsubscript{2} (black solid) and in presence of 1% H\textsubscript{2} (red dashes), (b) Experimental shift of LP_{0.10} resonant wavelength in presence of 1% H\textsubscript{2} at 70°C.

Fig. 9. Plot of effective indices of the first eleven cladding modes of the LPFG as a function of Pd layer thickness showing the transition region.
As a particular case, the simulated PMC and spectra for the LP$_{0.10}$ mode of an LPFG with period of 216 μm, for varying Pd layer thickness are shown in Fig.10. The LP$_{0.10}$ resonant wavelength as a function of Pd layer thickness is shown in the inset. The resonant band experiences a blue shift with increasing Pd thickness as the LP$_{0.10}$ effective index increases. The resonant band shifts rapidly with the Pd thickness between 10 to 16 nm. If the Pd layer thickness is further increased beyond the thickness for mode transition, the higher order mode approaches the original position of the lower order mode without any coating. This is the reason for the red shift of the LP$_{0.6}$ mode upon coating with a 60 nm thick Pd layer shown in Figs. 3 and 4. A Pd thickness of 60 nm is beyond the transition region and it is the higher order mode that appears slightly to the right of original position of the lower order mode. Fig. 11(a) shows the wavelength shift of the LP$_{0.10}$ mode of the aforementioned LPFG in presence of 1% H$_2$ (assuming a -5% change in real part and 5% change in imaginary part of the RI of Pd), for varying Pd layer thickness. The wavelength shift due to H$_2$ uptake increases with increasing Pd layer thickness between 8 to 15 nm. A wavelength shift of about 22 nm with ~15 nm Pd thickness may be achieved. The simulated LP$_{0.10}$ loss bands without H$_2$ and in presence of 1% H$_2$ for a 15 nm thick Pd layer are shown in Fig. 11(b).

The Pd layer not only acts as a sensitive layer for H$_2$ but also contributes in drawing out the evanescent field when its thickness is chosen to be in the transition region. As illustrated in [34], during the transition, the field content in the overlay, and so the interaction between the evanescent wave and the surrounding medium, reaches its maximum value. This is the reason for the high sensitivity of LPFGs coated with high index layers in the transition region. This is analogous to the role of sub-wavelength nanofilms in drawing out the evanescent field as reported in [35]. It has been reported in [36, 37] that metal oxide coated LPFGs lead to wavelength sensitivity enhancement compared to bare LPFGs.

Fig. 11. (a) Simulated wavelength shift for the LP$_{0.10}$ mode of the LPFG in presence of 1% H$_2$ with varying Pd layer thickness (b) Simulated LP$_{0.10}$ resonant loss bands in absence of H$_2$ (black solid) and in presence of 1% H$_2$ (red dashes) for the LPFG coated with a 15nm thick Pd layer.

D. Response of cladding modes at turn-around-point

The resonance between the core mode and a specific higher order cladding mode at turn-around-point (TAP) of its phase matching curve (PMC) produces a single broadband attenuation around the TAP. It is known that the sensitivity of a resonant mode to surrounding RI can be made appreciably high by designing the LPFG resonant mode around the TAP. In this section we present our simulated results that describe the sensitivity of a higher order cladding mode of a Pd coated LPFG operating around the TAP. Fig. 12a shows the PMCs of the LP$_{0.12}$ mode for an LPFG with Pd coatings of different thicknesses. The black solid line shows the PMC of the mode when there is no coating on the LPFG. It also shows that an LPFG with a period of ~ 167 μm will produce a single broad band at the TAP having a resonant wavelength at ~ 1.34 μm as shown by the solid black line in Fig. 12b. As may be seen from the Fig. 12b, the resonant band splits into two with increasing thickness of the Pd layer. The shifts of the two resonant wavelengths as a function of Pd layer thickness are shown in the inset. We limited our analysis up to 15 nm of Pd thickness because for this thickness and above, the resonant peak on the right of the TAP moves beyond 1600 nm and is not very useful for practical measurements due to the limitation of the broadband source. The same argument is valid for the resonant modes on the left of the TAP. The wavelength shifts of the left and right resonant bands in presence of 1% H$_2$ (assuming a -5% change in real part and 5% change in imaginary part of the RI of Pd) as a function of Pd layer thickness are shown in Figs. 13(a) and 13(b), respectively. The results clearly show that Pd layer thickness does influence the sensitivity.
The simulated left and right loss bands for the TAP-LPFG coated with a 13nm thick Pd layer, without H\textsubscript{2} and in presence of 1% H\textsubscript{2} are shown in Figs. 14(a) and 14(b), respectively as a particular example. The left loss band shifts by -6 nm, while the right loss band shifts by 12 nm. It may be seen that the loss band around 1550 nm can easily be monitored using standard SLED source but if a broadband white light source is used, measuring the separation between the loss bands is also possible where the wavelength shift for 1% H\textsubscript{2} adsorption will turn out to be around 18 nm.

The aim of the analysis presented in this paper is to understand the influence of thin Pd layer on the LPFG cladding modes. The analysis could estimate an optimum Pd layer thickness so as to operate the LPFG cladding mode around the highly sensitive mode transition region. There are available technologies to provide Pd layers of precisely controlled thickness and also technologies to produce appropriately designed LPFGs. We should mention at this point that it is too simplistic to dictate any specific combination of the % change in real part and imaginary part of the Pd layer RI in response to H\textsubscript{2} through this analysis.

IV. CONCLUSIONS

In this paper we present a detailed theoretical analysis regarding the response of cladding modes of metal coated long period fiber gratings (LPFGs) to changes in the thickness and complex refractive index (RI) of the metal coating. We have primarily focused our investigation for thin palladium (Pd) layers. To do this we have considered a four layer waveguide structure and used matrix method to model LPFG cladding modes with a layer of material having complex RI. We used Newton’s method to solve the complex characteristic equation and numerical integration to solve the coupled mode equations. To validate the model we compared our simulated results with experiments. Response characteristics of the cladding modes at the turn-around-point and also at mode transition have been investigated. This aspect has not been investigated in previous work on LPFG based hydrogen sensors. We show that if designed properly a thin layer of Pd can produce a highly sensitive hydrogen sensor. It is already mentioned that a thin Pd layer facilitates fast response and recovery. With the aid of the predictive model presented in this paper it will be possible to know the behavior of thin Pd layers in presence of hydrogen with systematic experiments. This is going to be our research plan in future with a target to produce ultrasensitive and fast LPFG based hydrogen sensors.

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