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Design of a metal hydride-coated tilted fibre Bragg grating-based hydrogen sensor

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ABSTRACT

Hydrogen, crucial in industrial and environmental realms, demands precise sensing methods. This study focuses on the design of a metal hydride-coated tilted fibre Bragg grating (TFBG) based sensor for hydrogen detection, introducing tantalum as a novel sensing material for fibre optic hydrogen sensor development. To facilitate the ellipsometry inspection of optical constants, magnetron sputtering technique has been employed to deposit nanometer-scale metal films onto a glass substrate. Numerical modeling results are presented for mode analysis of the proposed sensor design, analyzing transverse mode behavior for sensor optimization. The study also provides insights into other TFBG sensor design considerations, suggesting potential hydrogen sensing applications, such as hydrogen-powered aviation and storage solutions.

Keywords: hydrogen sensors, fibre optic sensors, tilted fibre bragg grating, metal hydrides

1. INTRODUCTION

Hydrogen, with its high potential as a near zero carbon emission fuel, plays a critical role in diverse industrial and environmental applications in the transition to clean energy sources from fossil fuel. Consequently, precise and dependable sensing methodologies are essential for effectively monitoring its presence and concentration to ensure safe operation. Fibre optic sensors have gained prominence in hydrogen detection, owing to their inherent benefits, including enhanced sensitivity, spark free operation, immunity to electromagnetic interference, and remote sensing capabilities.[1]

Among various fibre optic sensor configurations reported in hydrogen sensing, such as micro-mirror[2] and surface plasmon resonance (SPR)[3] based fibre optic sensors, tilted fibre Bragg grating (TFBG) based hydrogen sensors[4,5] have emerged as high-performing candidates due to their heightened sensitivity to external refractive index (RI) variations. When a TFBG is combined with a suitable metal hydride, one can use it to construct a hydrogen sensor. This metal hydride gradually absorbs hydrogen when hydrogen is present near the material, inducing a gradual change of the optical properties of the material.

While palladium (Pd) has been videly explored as a potential hydrogen sensing material in collaboration with fibre optic sensors,[1,6] it exhibits hysteric behavior due to phase transition that occurs upon exposure to 1-10% hydrogen concentration. Recently, we have reported tantalum (Ta) as a novel, emerging, high-performing candidate to overcome these challenges associated with Pd in hydrogen sensing.[7,8] This study focuses on exploring the design of Ta metal hydride-coated TFBG sensors, leveraging the advantages of both Ta and TFBGs.

To systematically design a fibre optic hydrogen sensor based on a TFBG and this novel material, we first establish and present their optical constants through ellipsometry. This is achieved by depositing a nanometer-scale thin film stack of metals, which serves as the adhesion, sensing, and capping layer, onto a glass substrate using magnetron sputtering. The coating process assumes fundamental importance as it enables the selective absorption and desorption of hydrogen molecules, leading to discernible alterations in optical properties.

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Subsequently, by integrating these optical constants into a numerical model, behaviour of cladding mode resonances of the Ta coated TFBG sensor are explored. Key parameters such as the electric field profile of transverse modes, effective refractive indices, and mode field diameters are analysed and presented.

Beyond mode analysis, this study also investigates the effect of grating parameters such as tilt angle, length and cladding diameter on the cladding mode resonances in designing the Ta based TFBG hydrogen sensor. This innovative design approach, combining efficient Ta-based metal hydrides with TFBGs, opens new avenues for the development of optical hydrogen sensors tailored to diverse applications, including hydrogen-powered aviation and hydrogen storage solutions.

2. SENSING PRINCIPLE

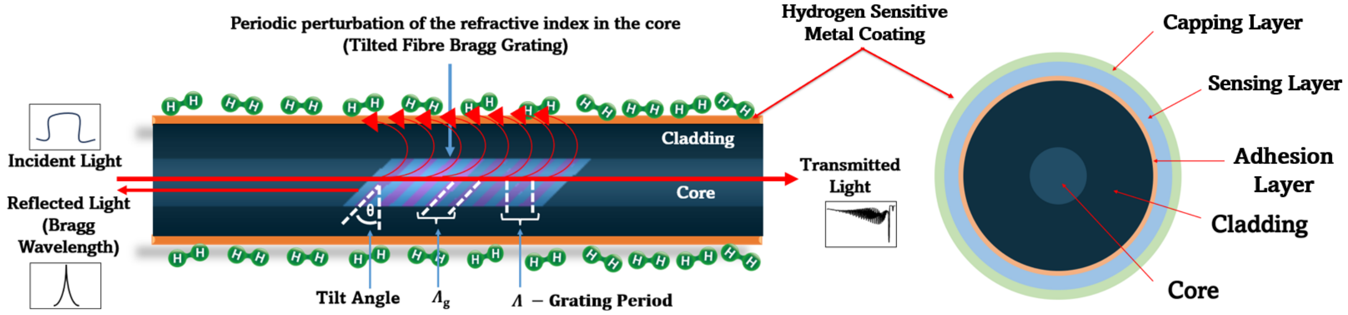

Figure 1: Schematic of the designed fibre optic sensor

Figure 1 illustrates the schematic of a metal-hydride based TFBG fibre optic hydrogen sensor. The sensing metal layer stack (deposited on the cladding of the TFBG) consists of three layers: a 5 nm titanium (Ti) layer for improved adhesion between the Ta layer and the SiO_2 glass surface, a 50 nm Ta sensing layer sandwiched between the Ti layer and a 15 nm $Pd_{0.6}Au_{0.4}$ capping layer. The capping layer serves dual purposes: protecting the Ta layer from oxidation and catalyzing in the dissociation of hydrogen molecules into individual atoms. As explained in Lars et al. (2020),[9] the metal layer stack absorbs hydrogen, forming metal-hydrides and altering its optical properties, particularly the RI. These changes in optical properties are translated into an optical signal by modifying the transmission spectrum of the Ta-deposited TFBG. The extent of these alterations depends on the RI of the Ta sensing layer, itself determined by the concentration of hydrogen in the surrounding environment. Thus, the characteristics of the TFBG transmission spectrum can be utilized to measure and quantify the hydrogen concentration in the surrounding environment. The Bragg wavelength of the TFBG, λ_{Bragg}, can be defined as below.[10]

$$\lambda_{Bragg} = [n_{eff}^{core}(\lambda) + n_{eff}^{core}(\lambda)]\Lambda_g/cos\theta \tag{1}$$

Individual cladding resonances of the TFBG transmission spectrum can be defined by;[11]

$$\lambda_{clad,i} = [n_{eff}^{core}(\lambda) + n_{eff,clad}^{i}(\lambda)]\Lambda_g/cos\theta \tag{2}$$

and the reflectivity (R) or the strength of the individual cladding mode resonances can be defined by;[10]

$$R = tanh^2(kL) \tag{3}$$

where $n_{eff}^{core}(\lambda)$ is the effective RI of the core mode, $n_{eff,clad}^{i}(\lambda)$ is the effective RI of the i^{th} order cladding mode, λ is the wavelength, θ is the tilt angle, and Λ is the period of the TFBG structure. L is the length of the TFBG and k is the coupling coefficient between the core mode and the i^{th} order cladding mode. As can be seen from equation (2), the resonance wavelengths of a thin film coated TFBG is a function of $n_{eff,clad}$, which comprises of the cladding RI, as well as the RI index of the coated thin film layer, in this case, Ta based metal sensing layer stack. When the Ta coated region of the TFBG absorbs hydrogen, the RI of the sensing layer changes, which leads to pertubations in the centre wavelength and the amplitude of the respective resonance loss bands. This forms the sensing principle of the Ta thin film coated TFBG sensor designed in this work.

3. RESULTS AND DISCUSSION

3.1 Ellipsometry Results

To investigate the optical constants/RI of the sensing layer, the described metal layer stack was deposited onto a quartz substrate sized 10 × 10 × 0.5 mm^3 using magnetron sputtering. Please consult our previous research for detailed information on the deposition procedures.[8] Optical constants of each material were measured via spectroscopic ellipsometry (Woollam M-2000) across the wavelength range of 210 nm - 1690 nm (angles varied from 45° to 65°). Figures 2 and 3 depict the optical constants of the adhesion layer (Ti), the sensing layer (Ta), and the capping layer ($Pd_{0.6}Au_{0.4}$) measured at room temperature.

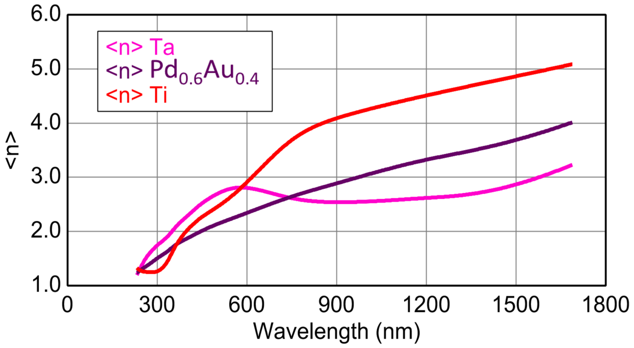

Figure 2: Real part (n) of the refractive index

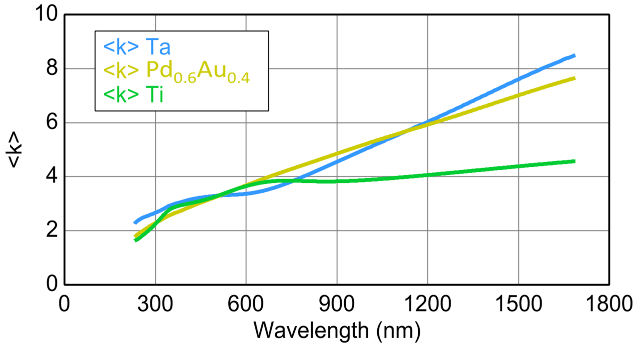

Figure 3: Imaginary part (k) of the refractive index

3.2 Mode Analysis

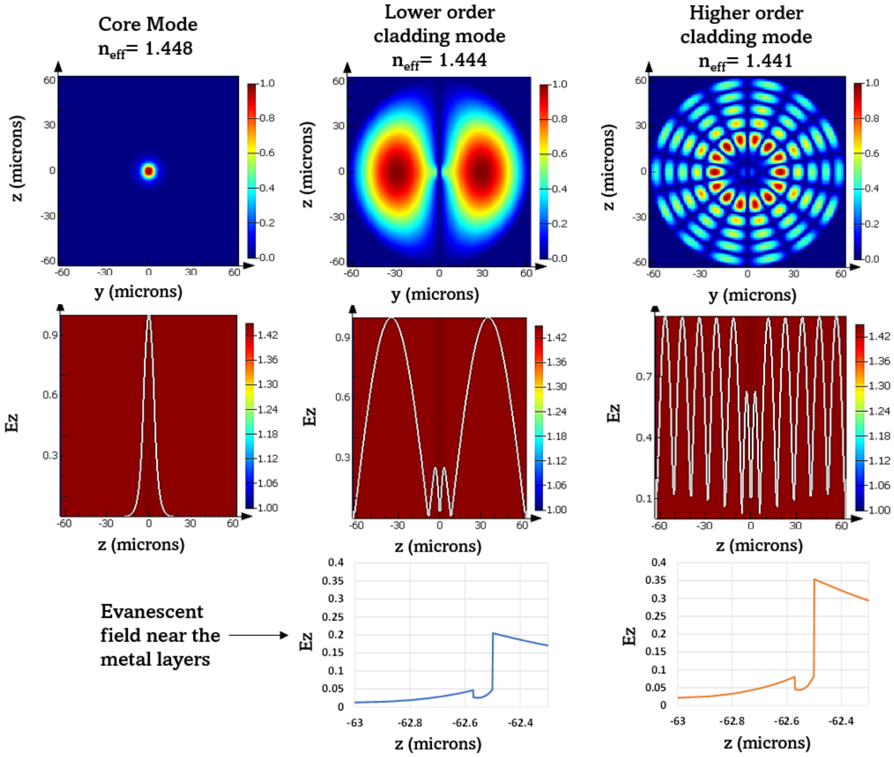

Figure 4: Mode behaviour of the Ta coated TFBG

The measured optical constants of the sensing layer were employed as inputs for the numerical model used to analyse the mode characteristics of the TFBG sensor. A numerical model utilizing the Bidirectional Eigenmode Expansion method in the frequency domain (ANSYS Lumerical) was utilized for analysing modes and electromagnetic wave propagation. A standard single-mode optical fibre with a core RI of 1.45 and a cladding RI of 1.445, with a core diameter of 4.1 µm and a cladding diameter of 62.5 µm, was considered. For the grating, a RI modulation of 0.0003 was taken into account. The operating wavelength considered was 1550 nm. Figure 4 depicts the transverse electric field profiles of the fundamental core mode, a lower order cladding mode, and a higher order cladding mode. Evanescent field plots near the metal layers on the cladding surface show that the higher order cladding modes interact more with the sensing metal layer compared to the lower order cladding modes. This implies that higher order cladding modes are more sensitive to RI changes in the sensing layer. As a design consideration, increasing the number of higher order cladding modes realized from the TFBG would enhance the sensitivity of the designed TFBG sensor. The next section elaborates on how this can be achieved.

3.3 Design Considerations

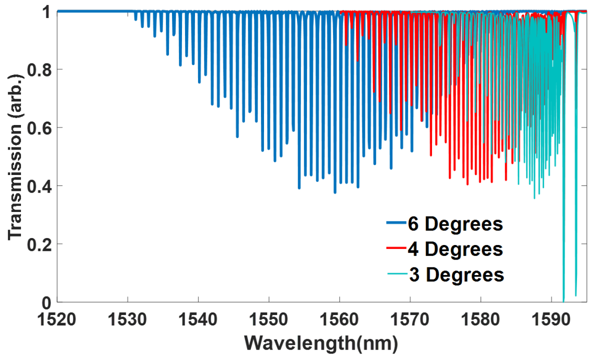

Figure 5: Effect of tilt angle on cladding mode envelope

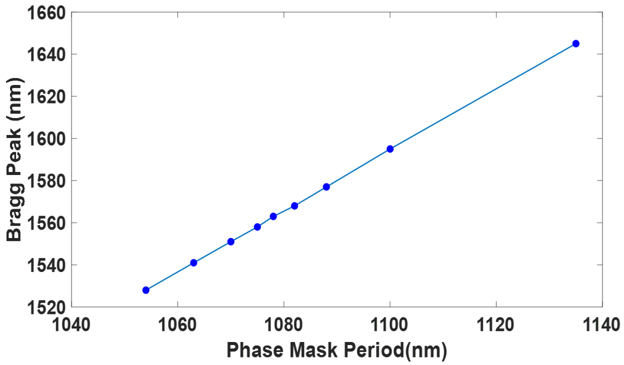

Figure 6: Effect of the grating period on λ_{Bragg}

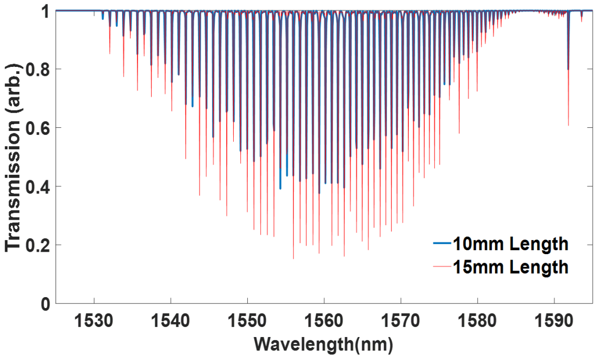

Figure 7: Effect of TFBG length on transmission spectrum

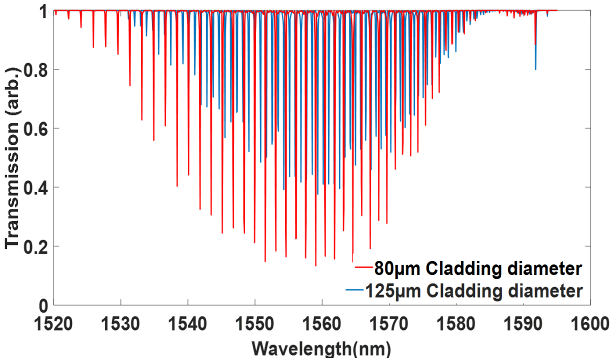

Figure 8: Effect of reduced cladding diameter on transmission spectrum

Figure 5 illustrates the evolution of the cladding mode envelope with an increasing tilt angle of the grating plane of the TFBG. Observing the cladding mode resonances, it's evident that higher order cladding modes can be coupled to the core mode by increasing the tilt angle. By substituting the effective RI of the fundamental core mode found via the numerical model in the previous section into equation (1), the center wavelength of the Bragg peak was calculated for different available phase masks (assuming the grating period is 0.5 times the period of the phase mask). These values are depicted in Figure 6, where Bragg peak indicates the upper limit of the TFBG transmission spectrum. Our fibre optic interrogator (National Instruments PXIe-4844) operates within a wavelength range of 1510 nm to 1590 nm. Taking into account the aforementioned design considerations, a 1100 nm phase mask (corresponding to a 550 nm grating period) and a 6-degree tilt angle were chosen to achieve the most optimal cladding mode envelope within the 1510 -1560 nm wavelength range. Figure 7 demonstrates that the strength (amplitude) of cladding mode resonances can be enhanced by increasing the length of the grating.

This relationship is also evident from equation (3). Additionally, Figure 8 illustrates the effect of the cladding diameter on the cladding resonances. It is observed that as the cladding diameter decreases, the amplitude of cladding mode resonances increases while the spacing between each resonance also increases.[10] This suggests that by reducing the cladding diameter, the sensitivity of the sensor can be heightened, while making it easier to interrogate individual cladding resonance peaks. The grating parameters discussed, along with the mode analysis, emphasize the factors considered in designing the Ta-based TFBG hydrogen sensor.

4. CONCLUSION

A Ta metal-hydride coated TFBG sensor has been designed, considering optical constants of the sensing layer and TFBG grating parameters. Higher order cladding modes exhibit enhanced interaction with the metal hydride layer. This improved interaction is facilitated by higher tilt angles, allowing a greater number of cladding modes to couple with the fundamental core mode. An optimal 6-degree tilt angle was identified, maximizing the coupling of cladding order modes to the core mode within the operating wavelength range of 1510 nm to 1590 nm, as determined by the fibre optic interrogator. If necessary, the cladding diameter can be chemically reduced to increase the sensitivity of the proposed TFBG hydrogen sensor. The next step involves realizing and testing the performance of the designed Ta based TFBG sensor for detecting various hydrogen concentrations.

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