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15

Numerical modeling of the propagation constant in a Pd-coated integrated optical waveguide as a function of atmospheric hydrogen concentration

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In this paper the possibility of hydrogen detection using waveguide structures based on SiN with a thin Pd film deposited on the cladding surface is considered. The dependence of the propagation constant and optical power transmission coefficient on the geometric parameters of the configuration and hydrogen concentration was investigated using numerical modeling methods.

Keywords: silicon nitride, hydrogen, photonic sensor.

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Hydrogen is one of the important reagents in the chemical industry. Gas H_2 is used as a reducing agent in the production of ammonia and hydrochloric acid. Since combustion of H_2 produces only water vapor, hydrogen has been considered in recent years as an environmentally clean fuel for automotive and aerospace industries [1].

H_2 is a colorless and odorless gas, which significantly complicates the detection of its leaks. At the same time, H_2 is explosive in concentrations ranging from 18% to 59% when mixed with air; the flammable concentration range is from 4% to 75%; H_2 also has a low ignition energy ($20\,\mu$J) and high heat of combustion (285.8 kJ/mol) [2,3].

Today, hydrogen detection is addressed using electrical sensors, among which the following classes can be distinguished: electrochemical, metal-oxide, catalytic, and sensors based on detecting changes in thermal conductivity [3]. The common drawbacks of the listed sensor classes stem from their use of electrical signals, making these sensors potentially vulnerable to electromagnetic interference and posing a spark generation hazard [1].

An alternative to electrical hydrogen sensors are optical sensors, which use safe and interference-immune signals. Currently, optical fiber (OF)-based hydrogen sensors are known [2–5]. A disadvantage of OF sensors is the need for complex technological processing of OF (including etching and deposition of metal and dielectric nanolayers) to form sensors, as well as design limitations associated with the standardization of OF geometric dimensions. Using photonic integrated circuits (PICs) as sensing elements appears a simpler task, as modern photonics has numerous technologically mature platforms suitable for this purpose.

The standard scheme of a chemical (or biological) optical sensor is a Mach–Zehnder interferometer (MZI), in which one arm is stripped of cladding [6]. For gas detection, such a scheme is unsuitable because it lacks selectivity for a specific gas type. As a prototype, consider a device based on OF with a thin Pd film deposited on its cladding, through which hydrogen exposure changes the Bragg wavelength of the grating formed inside the optical fiber. To register changes in the Bragg wavelength, an optical spectrum analyzer is used in this configuration. Transitioning from optical fiber to thin-film waveguide structures will enable sensing element configurations where detection can be performed at a fixed wavelength, simplifying and reducing the cost of the sensor system. This detection capability is based on the fact that if an integrated optical waveguide is loaded with a thin Pd film, the propagation constant of optical radiation in the waveguide will depend on the optical characteristics of the Pd film. If this change occurs in isolated way, for example, in one arm of a Mach–Zehnder interferometer or directional coupler, it will lead to a change in optical power at the output of the optical element. The hydrogen concentration affecting the thin Pd film can be determined from the magnitude of the optical power change.

Thus, the purpose of this work is numerical modeling of the dependence of the propagation constant of optical radiation in an integrated-optical waveguide loaded with a thin Pd film on hydrogen concentration in the atmosphere.

Consider an integrated-optical waveguide on which a thin Pd film is deposited on the cladding surface, with physical properties changing under H_2 exposure.

This work considers waveguides based on silicon nitride SiN on SiO_2insulator, since the relatively low refractive index contrast between SiN and SiO_2 provides weak optical field confinement in the waveguide core, allowing

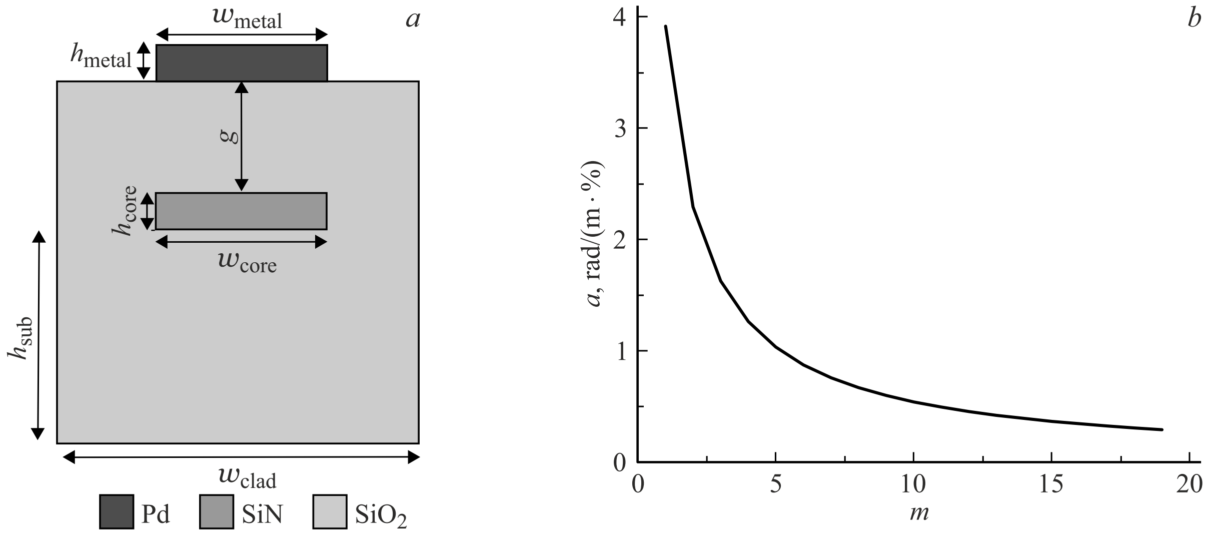

Figure 1. Waveguide cross-section and dependence of parameter a on parameter m.

Designation	Parameter	Value
h_{sub}	Substrate height	$2.5\,\mu$m
w_{clad}	Cladding width	$5\,\mu$m
h_{core}	Waveguide core height	160 nm
w_{core}	Waveguide core width	$1.4\,\mu$m
g	Distance between core and cladding surface	$1\,\mu$m
h_{metal}	Pd strip height	50 nm
w_{metal}	Pd strip width	$1.4\,\mu$m
–	Waveguide length	$5\,\mu$m
λ	Optical radiation Wavelength	$1.55\,\mu$m

stronger interaction of optical radiation with the external environment. Note that the abbreviation SiN is used in the text, as the exact stoichiometry of the silicon nitride deposited on our equipment using PECVD is unknown; the correct stoichiometric formula is Si_3N_4 or close to it.

The model parameters are presented in the table. In the following, if one parameter varies, all others correspond to the values given in the table. Modeling was performed in COMSOL Multiphysics using the finite element method.

The values of h_{sub} and w_{clad} are model parameters limiting the size of the modeled domain. The value of h_{sub} corresponds to the thickness of the SiO_2 layer planned to be formed on the silicon substrate surface before SiN deposition. The modeled domain widthw_{clad} is dictated by computer computational power limitations; physically, SiO_2 will also be present beyond the right and left model boundaries. Scattering boundary conditions were set at the external model boundaries to prevent reflection of optical radiation back into the modeled domain.

The refractive index of air was taken from data in [7], hydrogen from [8], SiO_2 — from [9], SiN from [10]. The relative dielectric permittivity ε_{Pd} depending on hydrogen concentration is determined by the expression [4, 5]:

$$\varepsilon_{\text{Pd}}(C_{\text{H}_2}) = h(C_{\text{H}_2}) \cdot \varepsilon_{\text{Pd}}(0), \tag{1}$$

where $h(C_{\text{H}_2}) \leq 1$ — is an empirically derived nonlinear function determining the decrease in dielectric permittivity of the thin Pd film with increasing C_{H_2}. Since the form of this dependence is unknown, it was decided at this stage to adopt:

$$h(C_{\text{H}_2}) = \frac{1}{1 + C_{\text{H}_2}/(m \cdot 100\%)}, \quad m > 0. \tag{2}$$

This dependence may be revised in the future if experiments reveal a different form. The dielectric permittivity values, real and imaginary parts of the refractive index of the thin Pd film were taken from [11].

To assess the efficiency of hydrogen impact on the propagation constant, least squares approximations of β dependences on C_{H_2} were constructed for varying geometric parameters. The approximation equation had the form

$$\beta = a \cdot C_{\text{H}_2} + b, \tag{3}$$

where a is the slope coefficient with dimensions$\frac{\text{rad}}{\text{m}\cdot\%}$, b is a constant with dimensions rad/m.

Note also that this work considers propagation of the horizontally polarized optical mode TE_0 as only this mode can propagate in the waveguide with the specified parameters in the absence of Pd.

Fig. 1, a shows the cross-section of the considered waveguide. The dependence of a on m is shown in Fig. 1, b.

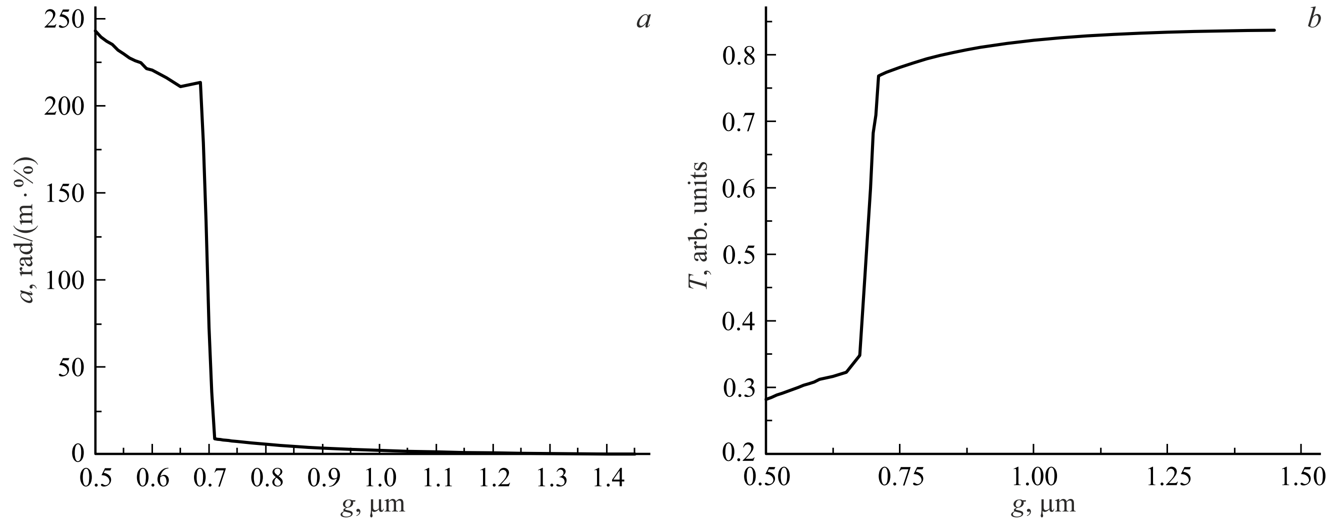

Figure 2. Dependence of parameter $a$and transmission coefficient on parameter g.

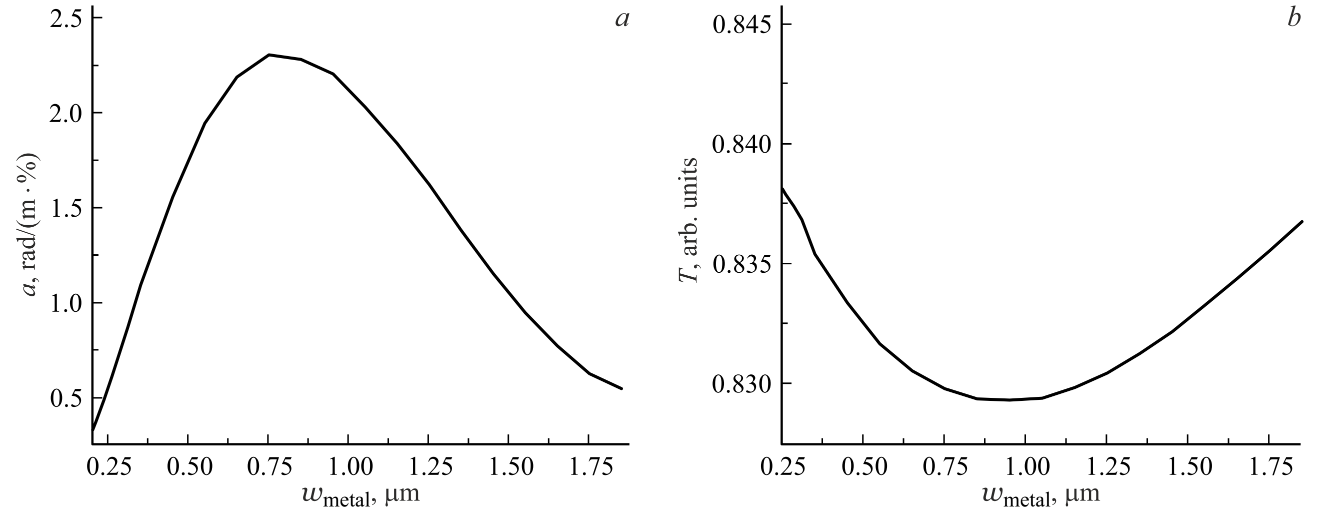

Figure 3. Dependence of parameter a and transmission coefficient on parameter w_{metal}.

All subsequent dependences will be plotted at $m = 4$. The choice of $m = 4$ is due to the fact that at this value, modeling can be performed with a hydrogen concentration sweep step of 0.1%, reducing computation time compared to smaller values while ensuring sufficient change in the propagation constant with varying model geometric parameters, simplifying result analysis.

Fig. 2 shows the dependences of a on g and transmission coefficient T for waveguide length$5\,\mu$m on g.

Fig. 3, a shows the dependence of parameter a on the metal strip width on the waveguide cladding surface (w_{metal}), Fig. 3, b shows the waveguide transmission coefficient dependence for length $5\,\mu$m on w_{metal}.

Similarly, Fig. 4 shows the dependence of a on Pd film thickness (h_{metal}).

As seen from Figs. 2–4, parameter a has the greatest impact on both the transmission coefficient and parameter g. The figures indicate that g values below $0.75\,\mu$m provide too small transmission coefficients. The minimum acceptable g value is on the order of $0.75{-}1\,\mu$m. The $0.75\,\mu$m boundary arises due to the mode field diameter propagating in the waveguide with the configuration specified in the table and Fig. 1.

Thus, numerical modeling of the dependence of the propagation constant of optical radiation in an integrated-optical waveguide loaded with a thin Pd film on hydrogen concentration in the atmosphere was conducted. It can be concluded that sensing elements for hydrogen detection can be implemented based on integrated waveguide structures. The change in dielectric permittivity of the thin Pd film under hydrogen exposure leads to a change in the propagation constant in the waveguide with the Pd film deposited on its cladding. This propagation constant change can be converted to optical intensity change if

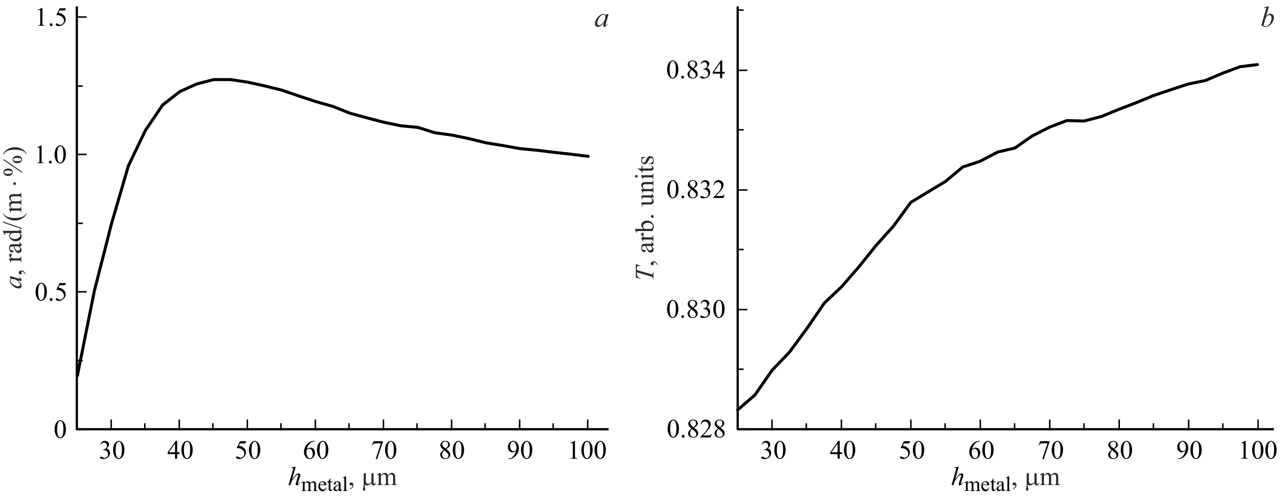

Figure 4. Dependence of parameter a and transmission coefficient on parameter h_{metal}.

used in Mach–Zehnder interferometer, integrated optical ring resonator, or directional coupler configurations. Then, hydrogen concentration changes can be analyzed from changes in PIC optical transmission at a fixed wavelength or from changes in optical transmission dependence when varying wavelength at fixed power level. Further work on sensing element development will primarily involve finding the optimal g value, as its variation has the greatest impact on both hydrogen sensitivity and optical transmission. Changes in the other considered parameters have significantly less impact on both the a value and waveguide optical transmission.

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Conflict of interest

The authors declare that they have no conflict of interest.

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