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Detection of propane gas adsorbed in a nanometer layer on silica nanowire

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ABSTRACT

In the present work, a miniature optical gas sensor for the leakage detection of propane is proposed. It is constructed by employing single mode silica nanowire Mach–Zehnder interferometer (MZI). Suitable chemical treatment of silica nanowire for propane gas adsorption onto it is suggested. In the proposed sensor, the idea is that, the propane gas gets adsorbed on treated surface of silica nanowire, which changes the refractive index of few nanometer thick layer on the nanowire surface. In theoretical modeling and simulation, full vectorial analysis of two and three layers tightly guiding waveguide structures are presented. Simulations include calculation of phase difference at the output end of MZI, phase sensitivity, detection limit and measurable refractive index over a practicable sensing length such as 1 mm. Sensing characteristics are numerically investigated. The sensor shows merits over conventional gas sensors. The sensing characteristics show negligible dependence on temperature, vibration and humidity, which is discussed in details. The proposed gas sensor is featured by high sensitivity, low cost, low loss, miniaturize size, and shows possibility of early detection of leakage.

1. Introduction

Gas sensing technology has recently gained much attention since the demand for low cost and highly sensitive gas sensors has increased for clinical, environmental, health and safety based applications. Reported gas sensors show wide variety of designs having attractive features, and detection mechanisms, some of which are built as the integrated devices. They show high sensitivity, miniature size and complex structures.

The optical gas sensors developed so far are broadly of two types, i.e. refractometric sensors or the absorption sensors. The refractometric sensors sense variations taking place in external refractive index due to presence of analyte gas in the external medium. In absorption sensors, the field gets absorbed in the sensing film due to absorption of analyte gas in sensing film. Other absorption sensors are based on fluorescence characteristics of sensing film, some of them are the dye based sensors.

The refractometric sensors with novel designs have been reported. These include humidity sensor, which shows good temperature immunity [1], state-of charge monitoring sensor [2], which uses quantum dots coupled to optical fiber. It shows a fast response and reasonable detection limit [3]. The others are based on fluorescence characteristics [4], surface plasmon resonance in the periodic grating structures [5], heterostructures [6] or infra-red cameras [7]. Some are the nanowire based sensors [8]. These sensors show high sensitivity, selectivity, low power consumption, and fast response. The dye based or sensors employing infra-red cameras need human monitoring. Wavelength selection is also not on hand, since it depends upon optical characteristics of the sensing medium. The sensors built as integrated devices use various waveguide devices such as planar waveguides [9], Mach–Zehnder interferometers [10], grating structures [11], fiber loop resonators [12], directional couplers [13], etc. Some of them show high sensitivity, selectivity, but composite structures. Hence fabrication cost is high. The dependence of sensing characteristics of some of these sensors on the external parameters such as humidity, temperature, and vibration also puts limitation on their application. Thus, industries, laboratories and households need low cost, compact, better performing and highly sensitive sensor devices.

In the present work, a simple and low cost propane gas sensor is proposed. It employees single mode silica nanowire Mach–Zehnder interferometer (MZI) as the waveguiding device. It is found in this work that silica nanowire shows a discontinuity and increased field amplitude at core–cladding interface, which is useful in sensing a few nanometer thick layer formed on the interface, with high sensitivity. It is known that silica nanowire can be fabricated by

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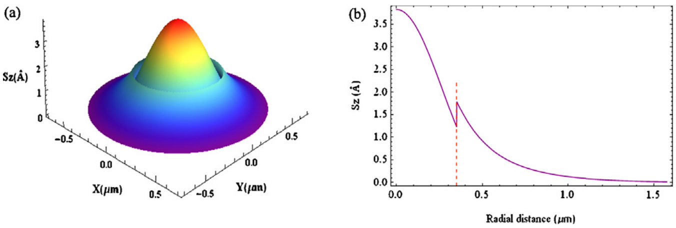

Fig. 1. Power profile for the air-clad single mode silica nanowire at 1.55 μm wavelength.

simple and low cost, high temperature fiber drawing technique. The fabricated nanowire shows excellent diameter uniformity, surface smoothness and good mechanical strength [14]. The reported scattering loss is as low as 0.0014 dB/mm [15]. Silica nanowire is identified as the potential candidate for building integrated devices. In the present work, for the first time, the use of single mode silica nanowire for propane gas sensing is proposed. Unlike other gas sensors which need fabrication technology, present propane gas sensor is simple in construction, functionalization, and operation. Simultaneously, it shows the benefits such as high sensitivity, low detection limit, reversibility and possibility of early detection of gas leakage.

The work is presented as follows. First, single mode silica nanowire is simulated for sensing a mono or multimolecular layer. Functionalization of silica nanowire surface for propane gas adsorption is discussed in detail. Simulations are performed to calculate phase difference, phase sensitivity, detection limit, minimum measurable refractive index and measurable refractive index over a practical sensing length such as 1 mm. Results and sensing characteristics, are discussed and conclusions are presented in the end.

Propane gas is highly flammable. Under the condition of gas leakage, it forms explosive mixtures with air, resulting in an explosion and toxicity hazard to the living beings. Since it is a widely used gas in industry for various processes and applications, in civil society in the form of vehicles, households and laboratories, its early detection is important. Present work gives a highly sensitive, simple to construct and a low cost device for propane gas detection.

2. Materials and methods

2.1. Waveguidance in silica nanowire

Proposed gas sensor being refractometric sensor, wavelength selection is on hand. Present sensor is designed to work at 1.55 μm for the following reasons. At this wavelength, the nanowire shows grater evanescent field leading to higher sensitivity, as compared to the lower wavelength such as 633 nm. This being the standard telecommunication wavelength, good quality light sources and detectors are available. Silica nanowire is well studied and improved for low loss operation, at this wavelength.

First, waveguiding characteristics of air-clad silica nanowire at 1.55 μm wavelength are studied. The power plot is obtained as shown in Fig. 1(a) and (b). The air-clad silica fiber has refractive index of 1.4468 at 1.55 μm wavelength. The infinite external medium is air. The air-clad nanowire exhibits tight light confinement. For obtaining the power plot, the dispersion equation given by Eq. (1) is numerically solved in order to obtain propagation constant (β) [16]:

$$\left(\frac{J_n'(u)}{uJ_n(u)}+\frac{K_n'(w)}{wK_n(w)}\right)\left(\frac{J_n'(u)}{uJ_n(u)}+\left(\frac{n_1}{n_2}\right)^2\frac{K_n'(w)}{wK_n(w)}\right)$$
$$=n^2\left(\frac{1}{u^2}+\frac{1}{w^2}\right)\left(\frac{1}{u^2}+\left(\frac{n_1}{n_2}\right)^2\frac{1}{w^2}\right) \quad (1)$$

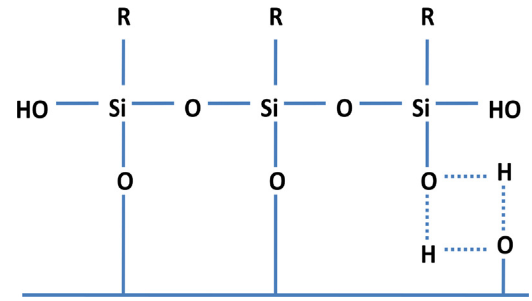

Fig. 2. Bond formation in silation process.

In this expression, u and w are the transverse wave numbers in core and cladding regions, given by $u=a\sqrt{k^2n_1^2-\beta^2}$ and $w=a\sqrt{\beta^2-k^2n_2^2}$, respectively, and a is the core radius. n_1 and n_2 are the refractive indices of core and cladding, respectively. k is the wave vector and β is the propagation constant. The quantities u, w and β are expressed in μm^{-1}. n represents mode number. Single mode silica fiber exhibits only fundamental HE_{11} mode, for which n is equal to 1. J is the Bessel function of first kind and K is the modified Bessel function of second kind.

Single mode cut-off condition for the air-clad silica nanowire is calculated as 1135 nm. Power profile for the air-clad single mode silica nanowire of 700 nm diameter is obtained by calculating the Poynting vector (S_z) (Å) as given in [16], and is plotted as shown in Fig. 1(a) and (b), by programming in Mathematica 7.0 software.

A field discontinuity and slightly increased evanescent field amplitude is observed at the core–cladding boundary in Fig. 1(b). The discontinuity originates from the discontinuity of transverse field components at the core–clad boundary. Due to this high field amplitude, sensing of a thin molecular layer on the core–clad boundary is possible. For this reason, it is proposed that a thin layer of gas adsorbed on the nanowire surface is detected.

2.2. Treatment of silica surface for propane gas adsorption

Since it is required that propane gas gets adsorbed on the nanowire surface, adsorption characteristics of propane gas on silica surface were studied and it was found that propane shows poor adsorption tendency on silica surface. It is found in literature that if silica surface is treated with methyl-hydrogen silane (or methoxysilane), the adsorption tendency improves. It is experimentally found to be the best adsorbent for propane gas [17]. The silane-treated silica surface obstructs adsorption of water and primarily adsorbs propane gas.

Silanes possess a hydrolytically sensitive center that can react with inorganic substrates such as glass or silica, to form stable covalent bonds. They possess an organic substitution that alters the physical interactions of treated substrates. The silane treatment is explained in detail in [18]. At the interface after treatment, usually one hydrogen bond exists between each silicon and the substrate surface as shown in Fig. 2. The two remaining silanol groups are present either in condensed or free form. The remaining R group is available for covalent reaction or physical interaction with other phases. The end-OH groups are replaced by methoxy group (CH_3) when treated with methoxy silane. The amount of silane used to silylate a surface decides the reactive sites formed on the surface, available surface area and formation of either a monolayer or multilayer or the bulk [19].

The surface bonds of silane treated silica have sufficient thermal stability to withstand short term process conditions of around 220 °C to 360 °C and long-term continuous exposure of 160 °C [20] and the surface substituted groups decompose at temperatures greater than 480 °C [17]. Thus, the treated surface is chemically