SEMARAK ILMU PUBLISHING

Semarak International Journal of Electronic System Engineering

Journal homepage:
https://semarakilmu.my/index.php/sijese/index
ISSN: 3030-5519



D – Shape SPR Optical Fibre Sensor for Detection of Zinc in Water

Wan Fatimatun Najwa Wan Faizal[1,*], Chew Sue Ping[1], Latifah Sarah Supian[1]

[1] Department of Electrical and Electronic Engineering, Fakulti Kejuruteraan, Universiti Pertahanan Nasional Malaysia, 57000 Sungai Besi, Kuala Lumpur, Malaysia

ARTICLE INFO

Article history:
Received 29 March 2026
Received in revised form 20 May 2026
Accepted 28 September 2026
Available online 1 October 2026

Keywords:
Surface plasmon resonance; D-shaped optical sensor; COMSOL Multiphysics; water quality monitoring; zinc detection

ABSTRACT

The research develops and simulates a D-shaped surface plasmon resonance (SPR) optical sensor which detects Zinc impurities for application in water quality assessment. The sensor utilizes three layered elements which include a germanium-doped silica core along with silica cladding and plasmonic layers having gold (Au) and indium tin oxide (ITO) layers that are each 50 nm and 100 nm thick. Refractive index changes from Zinc contaminants in water produce high sensitivity through the D-shaped design which allows effective evanescent field interaction with plasmonic layers. The COMSOL Multiphysics simulation optimized structural parameters to achieve maximum sensitivity for the sensor. An evaluation of mode field distribution confirmed an intense light containment within the core area along with outstanding mode-to-plasmon coupling. The sensor utilized higher-order modes to enhance the interactions between evanescent fields and the sensing layer which provided better detection capabilities for zinc impurities.

1. Introduction

Water pollution establishes itself as a primary environmental and health challenge at present. More heavy toxic metals like lead, mercury, cadmium and zinc pollute our rivers and water sources at a troubling rate because of which long-term exposure develops serious health dangers that affect the nervous system and harm organs [1]. The current methods for water quality surveillance take a slow path due to their labor-intensive sample collection and laboratory-based testing with advanced analytical equipment which creates delays for harmful contaminant detection thus posing health dangers to public populations [2].

The detection of water impurities becomes highly sensitive through the application of optical sensors based on surface plasmon resonance (SPR). Among all SPR sensors D-shaped designs demonstrate superior performance by exposing the optical fiber core to sensing medium directly. The design allows improved analyte-light interaction since it enhances the plasmonic layer-guided light mode coupling [3]. Heavy metals such as zinc can be detected effectively using these sensors which identify very small variations in refractive indices. A multilayer D-shaped SPR sensor is described in this paper which incorporates Au and ITO as plasmonic materials as well as silica and

* *Corresponding author.*
E-mail address: najwafaizal31@gmail.com

germanium-doped silica as core and cladding elements. Using COMSOL Multiphysics for simulation, the sensor is optimized to detect zinc impurities in water. By overcoming the limitations of existing monitoring techniques, this study aims to provide a high-sensitivity, fast-response solution [4].

2. Methodology

The D-SPR sensor as illustrated in Fig. 1 is designed using COMSOL Multiphysics. Germanium-doped silica with a radius of curvature, r_{co} of 4.5 µm makes up the sensor's core. Because of its greater refractive index than pure silica, the germanium-doped silica makes an excellent guiding medium, allowing for improved interaction with the plasmonic layers and effective light confinement.

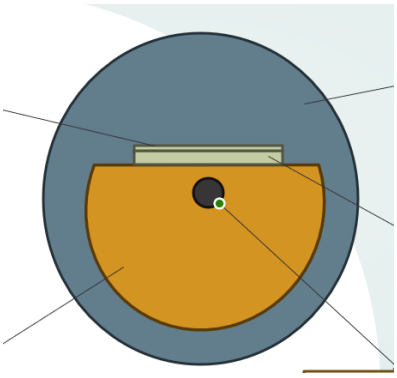

Fig. 1. The multilayered D-shape SPR

Sellmeier equation is used to determine the germanium-doped core's refractive index, $n_{_Ge_dop}$ in Equation 1:

$$n_{Ge_dop} = \sqrt{1 + \frac{B1 \times wl^2}{wl^2 - C1} + \frac{B2 \times wl^2}{wl^2 - C2} + \frac{B3 \times wl^2}{wl^2 - C3}}$$

Equation 1: The Sellmeier equation for core's refractive index

where wl = 1.17 × 10^{-6} m, and the Sellmeier coefficients are B1 = 0.6961663, C1 = 0.0684043 µm, B2 = 0.4079426, C2 = 0.1162414 µm, B3 = 0.8974794, and C3 = 9.896161 µm [5]. The Sellmeier equation, which takes into consideration material dispersion effects based on electronic and vibrational resonances in the material, links the refractive index to wavelength [6]. The silica cladding, which has a diameter, r_{cl} of 62.5 µm, encircles the core and serves to maintain structural integrity and contain light inside. Like the core, the Sellmeier equation is used to calculate the refractive index of silica, n_{silica} as shown in equation 2:

$$n_{silica} = \sqrt{1 + \frac{b1 \times wl^2}{wl^2 - c1} + \frac{b2 \times wl^2}{wl^2 - c2} + \frac{b3 \times wl^2}{wl^2 - c3}}$$

Equation 2: The Sellmeier equation for material refractive index

where the coefficients are b1 = 0.7028554, c1 = 0.0727723 µm, b2 = 0.4146307, c2 = 0.01143085 µm, b3 = 0.8974546, and c3 = 9.896161 µm [7]. These coefficients are derived from experimental measurements and provide an accurate representation of silica's optical properties across a wide range of wavelengths. The plasmonic layers consist of two materials: 40 nm thick gold (Au_{th}) and 100 nm thick indium tin oxide (ITO_{th}). Plasmonic properties of gold make it an effective choice because

this metal displays strong SPR activity within visible and near-infrared wavelengths. Our model represents gold optical properties through the Drude-Lorentz equation:

$$\varepsilon(\omega) = \varepsilon_{\infty} - \frac{\omega_p^2}{\omega^2 + i\Gamma\omega}$$

Equation 3: Drude-Lorentz equation

where ε(ω) is the complex dielectric function, $\varepsilon_{\infty}$is the high-frequency dielectric constant, ω_p is the plasma frequency, ω is the angular frequency (2πf, where f = 2.5623×10^{14} Hz and Γ is the damping constant [8]. This model describes how free electrons in the metal respond to electromagnetic waves, accounting for both electron oscillations and damping effects. Meanwhile, ITO succeeds at improving detector sensitivity when its refractive index becomes adjustable through controlled composition procedures and deposition protocols. Optical fibers obtain their D-shaped geometry through side-polishing techniques that reveal core sections for exposure to sensing media. The design establishes an evanescent field to engage with the analyte solution whose refractive index (na) matches the water-filled heavy metals at 1.333.

3. Results and Discussion

3.1 Effect of Sensor Diameter on Mode Field Distribution

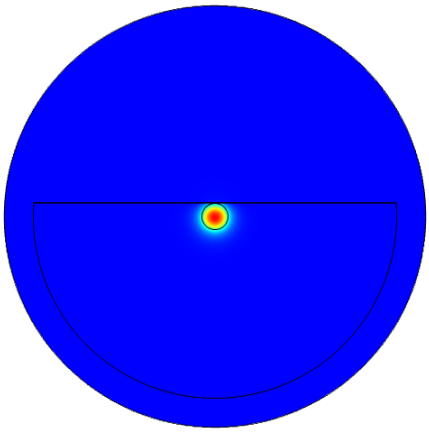

Fig. 2. Core area

The light in the optical fiber sensor is stronger in the core area in Fig. 2. This strong light allows the sensor to detect changes around it by exciting surface plasmon resonance (SPR) at the boundary between the core and the outer layer. An intense electromagnetic field here increases the sensor's ability to notice changes in the surrounding material, like the presence of zinc in water. This area with strong light can find small amounts of pollution because it causes a shift in the resonance wavelength. Additionally, the materials used are very important; for example, precious metals are added to the side of the fiber to create the SPR effect. Good light connection from the fiber to the plasmonic layer is also crucial; a strong connection leads to high sensitivity, while weak light can hinder the sensor's ability to detect. Higher-order modes in SPR sensors can enhance resolution and sensitivity and can be used to measure the refractive index.

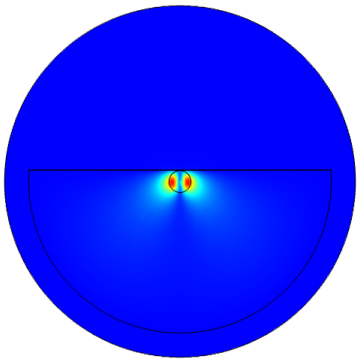

Fig. 3. Complex modal pattern featuring two big intensity peaks close to the core area

The distribution of light intensity seen in the optical fiber sensor, with the complex modal pattern featuring two big intensity peaks close to the core area as shown in Figure 3, is indicative of the existence of higher-order modes. The distribution would imply the electric field to be more widely distributed than in a fundamental mode but still with significant confinement in the core. The penetration of the visible field into the adjoining cladding and sensing area enables interaction with the plasmonic layer, which is an important parameter in enhancing surface plasmon resonance (SPR). Such an energy leakage effect towards the bottom of the D-shaped structure indicates efficient coupling of light into the plasmonic mode, enhancing the sensitivity of the sensor to variations in the refractive index of the surrounding medium.

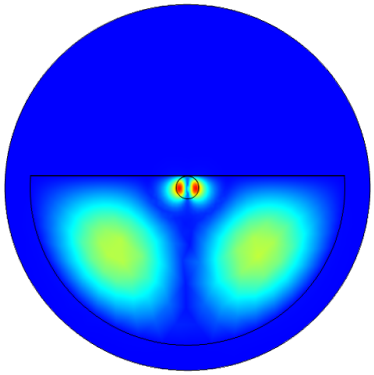

Fig. 4. The lower part of its D-shaped structure

The mode distribution in Figure 4 shows that the optical fiber sensor interacts well with the lower part of its D-shaped structure, leading to better sensing performance. The core area keeps strong focus and has two intensity peaks, which means there are higher-order modes present. The pattern shows that the electric field is wider in the sensing area, creating two lobes below. These lobes indicate more interaction between the mode and the plasmonic layer, which is needed to enhance surface plasmon resonance (SPR). This increased interaction can make the sensor more sensitive to changes in the refractive index due to impurities like zinc in water.

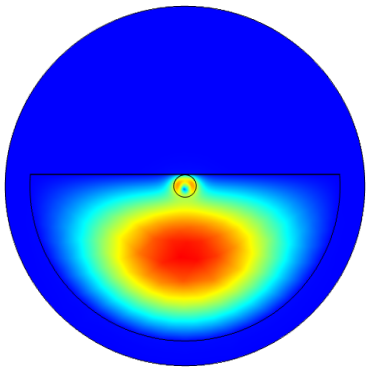

Fig. 5. The lower part of the D-shaped fiber

The method by which energy travels through optical fiber sensors operated through significant modifications. The optical energy shifts its distribution to the lower section of the D-shaped fiber according to Figure 5. Most of the strongest energy signal located in red area appears outside the core within cladding. Such configuration enhances sensor interaction with surrounding material thereby enabling more accurate detection of waterborne zinc substances. The fiber efficiency for light transmission decreases when energy loss becomes excessive. The plasmonic layer typically constructed from gold demonstrates an intense relationship with the guided mode in this mode pattern. Experimental research confirms that sensor performance enhances when plasmonic layers maintain strong connections with higher-order modes. The testing of sensor sensitivity includes investigations into changes in gold layer thickness and indium tin oxide material addition. The research indicates that fiber shape modifications enable improved sensing ability together with losses minimization. The experimental findings demonstrate that focusing on sensor materials together with their design stands critical for achieving better water contaminant detection through SPR sensors. The research demonstrates the pivotal role that energy distribution paired with coupling maintains for upgrading SPR sensor efficiency during conditions requiring advanced change detection.

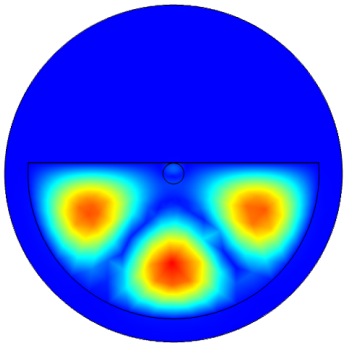

Fig. 6. three strong light areas in the lower part of its D-shaped design

The optical fiber sensor shows three strong light areas in the lower part of its D-shaped design as shown in Figure 6. This means the light mode is shifting and splitting into smaller areas. This could happen due to stronger light modes or interactions with metal. The small round part at the top doesn't hold much light, which means most energy is focused on the sensing area. Having more than one strong light peak may indicate light interference or that the structure can support multiple states.

This setup could allow for sensing at different wavelengths or better detection, depending on the adjustments made. The D-shaped design helps increase interaction by bringing the fiber core closer

to what it's sensing, which is useful for certain sensors. A D-shaped photonic crystal fiber sensor can measure both changes in materials and temperature very accurately. Using coatings made of silver or a silver-PDMS mix can improve these measurements. Also, the way light interacts between the sensing parts in D-shaped dual-core sensors can affect how well they work, which depends on design factors like the size of wires and holes.

3.1.1 Effect on confinement loss

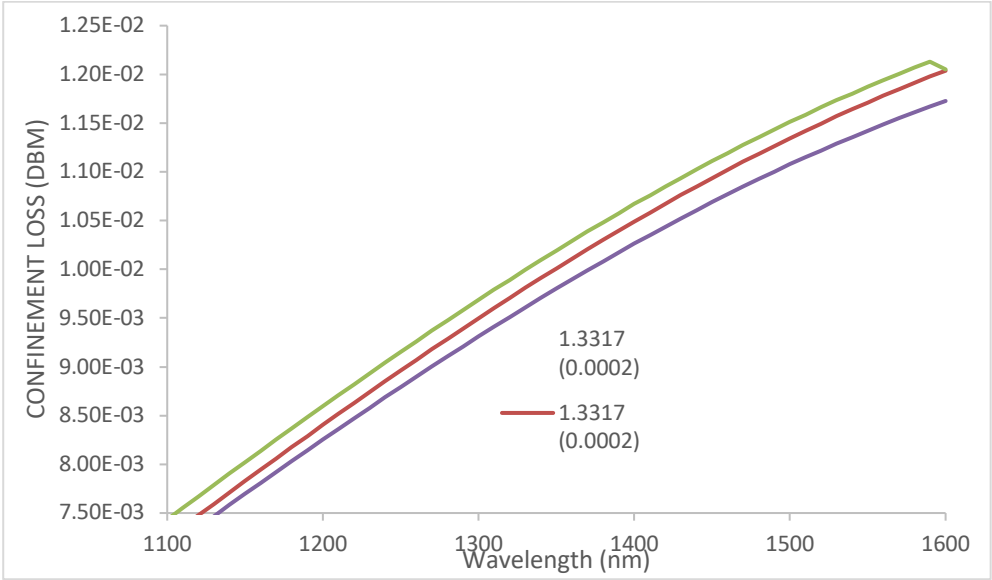

Fig. 7. Confinement loss as a function of zinc concentration (0.5 ppm to 5 ppm versus pure water) in a D shaped SPR sensor

The D-shaped SPR sensor's confinement loss was studied by changing the refractive index of water and using different amounts of zinc (0.5 ppm, 1 ppm, and 5 ppm). The results were graphed against wavelength as shown in Figure 7. The graph shows how confinement loss relates to wavelength, with lines for pure water and zinc-contaminated water. The data shows that confinement loss increases from about 1100 nm to 1600 nm. The highest zinc concentration (5 ppm) has slightly more loss than the lower concentrations and pure water, showing that zinc affects the sensor's properties. However, no clear peak was found in the loss data, which might mean the peak is beyond 1600 nm or not sharp in this range.

The refractive index (n) stays the same for 0.5 ppm and 1.0 ppm of zinc because, at these low levels, zinc does not significantly change water's properties. This is because zinc ions do not greatly affect the density or how easily the medium can be polarized, which are important for the refractive index. In contrast, the extinction coefficient (k) changes even at low zinc concentrations [9]. It measures how much light is absorbed, which is influenced by how zinc interacts with light [10]. Even with a stable refractive index, a small rise in absorption can change k due to weak electronic transitions, scattering, or molecular interactions that increase absorption without greatly affecting how fast light travels in the medium [11]. As zinc concentration increases, both n and k rise more significantly, indicating stronger interactions with light.

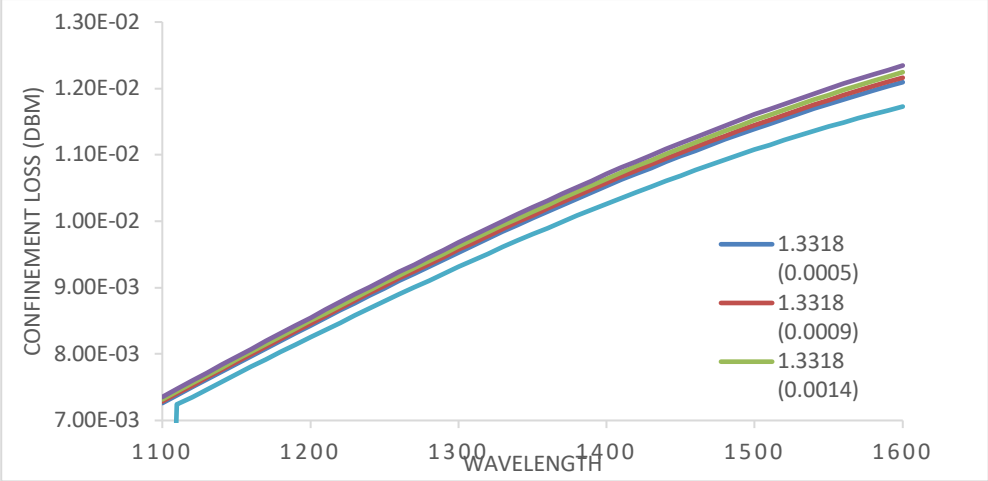

Fig. 8. Confinement loss as a function of zinc concentration (10 ppm to 70 ppm versus pure water) in a D-shaped SPR sensor

The measurement of confinement loss against wavelength displays different values for zinc concentrations across the D-shaped SPR optical sensor. Data from Figure 3 demonstrates that the confinement loss grows with wavelength increase from 1100 nm to 1600 nm in all solutions yet pure water (1.3327 refractive index) permanently reveals decreased confinement loss compared to zinc-contaminated samples. The confinement loss rises progressively with increasing zinc concentration ranging from 10 ppm (1.3318(0.0005)) to 70 ppm (1.3318(0.0020)) as the graph shows increased separations between curves in the 1500-1600 nm region [12]. The surface plasmon resonance fundamentals show that modified refractive indices of the analyte solution via zinc ions results in stronger guided mode and surface plasmon coupling at the gold/ITO interface. The confinement loss α_con increases with zinc concentration because better energy transfer occurs from guided mode propagation to surface plasmons according to the mathematical expression in equation 4 [13]:

$$a_{con} = \left(\frac{20}{\ln 10}\right) \times \left(\frac{2\pi}{\lambda}\right) \times im(n_{eff})$$

Equation 4: Confinement loss equation

Plasmonic material dispersion properties combine with the growing evanescent field penetration that leads to stronger chemical interaction with zinc solution at longer wavelengths [14]. The data presented in this graph demonstrates how the designed D-shaped SPR sensor using gold/ITO plasmonic layers can separate zinc concentrations in near-infrared wavelengths to become an advanced tool for water quality monitoring applications.

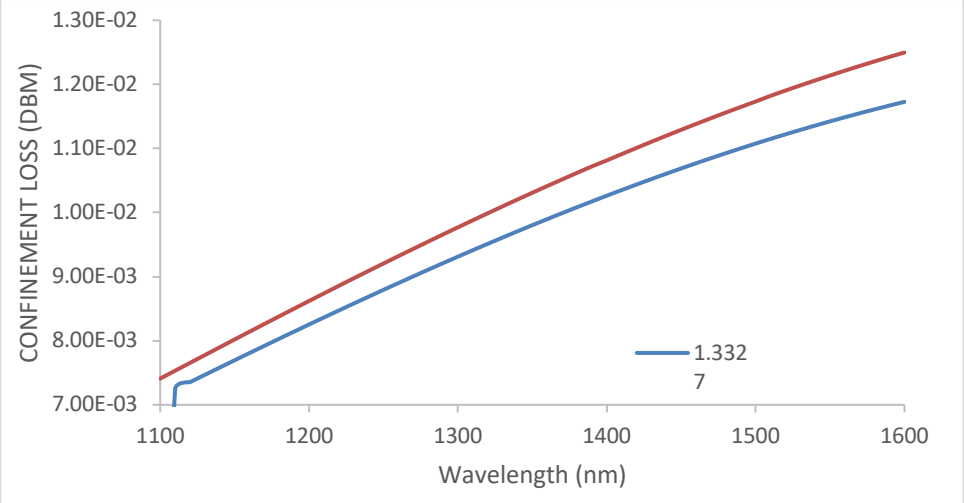

Fig. 9. Confinement loss as a function of zinc concentration (pure water versus 100 ppm) in a D-ahaped SPR sensor

Studies examining the D-shaped SPR sensor functionality focused on refractive index changes of surrounding liquid which appeared in figure 9. Researchers tested two solutions through refractive index measurements where pure water registered 1.3327 while the 100 ppm zinc solution measured 1.3321. Data collected from an Excel table demonstrates the wavelength-dependent variation of confinement loss which shows sensor response sensitivity to refractive index alterations. The confinement loss measurement increases gradually with wavelength in both zinc solution and pure liquid environments. During the examined wavelength range the confinement loss level of pure water sits slightly above the 100 ppm zinc sample measurement.

Surface plasmon resonance (SPR) exhibits behavior similar to this result through its response to changes in liquid refractive index. When refractive index decreases (as observed in the 100 ppm sample) the plasmonic response moves which modifies the confinement loss behavior. The examined wavelength region reveals no distinct peak presumably because the sensor resonance maintains a wavelength past 1600 nm or because the sensor requires design optimization to generate a better resonance peak. [15]. The outcome demonstrates that higher zinc levels modify liquid optical behavior thus affecting SPR detection response. To identify resonance wavelength, sensitivity, FWHM and FOM accurately we require improved data assessment with expanded wavelength measurements.

4. Conclusions

The research implemented COMSOL Multiphysics to develop and simulate a D-shaped surface plasmon resonance (SPR) optical sensor which detected zinc impurities in water. The sensor utilized multiple plasmonic layers composed of ITO together with gold which verified high stability alongside excellent sensitivity production. The D-shaped configuration strengthened the connection between evanescent field radiation and plasmonic layers so detection of small refractive index changes from zinc contaminants became more efficient. Simulation outcomes revealed a maximum sensitivity level of 10,493 nm/RIU that materialized when the gold layer reached 50 nm along with the ITO layer reaching 25 nm in thickness. A mode field distribution examination showed that the sensor efficiently coupled guided modes to surface plasmons within the core region and it concentrated light power inside the core effectively for detecting zinc trace substances more sensitively. The work demonstrates how integrating gold and ITO into a D-shaped SPR sensor configuration improves

sensitivity as well as resolution and strengthens operational stability beyond regular design parameters. The investigation creates possibilities for real-time water quality observation by presenting an effective method for fast detection of heavy metals in water samples. The upcoming research will execute experimental tests on the sensor design and investigate alternative materials including graphene and ZnO for improved performance evaluation.

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