



# Theoretical analysis of metamaterial-gold auxiliary grating sensing structure for surface plasmon resonance sensing application based on polarization control method

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## ABSTRACT

A metamaterial-gold multilayer sensing structure designed using the particle swarm optimization (PSO) algorithm with an auxiliary grating is proposed for using in a surface plasmon resonance (SPR) sensor system based on the polarization control method. After numerical calculations and simulation analysis, it was found that the metamaterial sensing structure significantly improves the sensitivity of the SPR signal with intensity singularity. The metamaterial sensing structure also increases the penetration depth of evanescent wave, making it possible to detect low-molecular-weight biomolecules and larger cells such as bacteria. The auxiliary grating structure was designed to identify the refractive index of the sensing region on both sides of intensity singularity. The stability of recognition and the electric field intensity of the visible light band were also studied.

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## 1. Introduction

Surface Plasmon Resonance (SPR) technology plays a significant role in fields of diagnostics, pharmaceuticals, food safety, and environmental monitoring [1–4]. It is a real-time and label-free method and can characterize and quantitatively detect low-molecular-weight compounds. One of the advantages of SPR sensors is their high sensitivity. However, the SPR technology still has limitations when detecting extremely low-molecular-weight biomolecules (<500Da) [5], such as proteins, hormones, and drugs, owing to their low polarizabilities, which result in a low resonance shift of the sensor. In addition, SPR biosensors can also be applied to biological analysis, such as detection of bacteria [6], receptor–ligand binding assays [7], and cancer diagnosis [8]. The penetration depth of an evanescent field, however, is restricted to between 200 nm and 300 nm. Furthermore, the evanescent wave is a type of attenuated electromagnetic wave in the medium of the system, and the diameters of biological molecules, including bacteria and proteins, are at the micron level. The SPR technology can only obtain information at the bottom or edge of the biological molecules in current applications [9]. Its applications in the analysis of biological molecules are therefore limited.

Veselago first proposed a metamaterial structure with negative permittivity and negative permeability [10]. Pendry proved the possibility of the existence of negative refractive index metamaterials, and

theoretically verified that metamaterials have an amplification effect on evanescent fields [11]. In 2012, Hujing demonstrated enhancement of sensitivity in a slab waveguide with TM mode and subwavelength resolution properties of a perfect slab lens, and the mechanisms of metamaterials for amplifying evanescent waves and for improving sensitivity and resolution were also studied [12]. In 2015, Upadhyay found that metamaterials could significantly increase the sensitivity of proposed four-layer reverse indexed profile waveguides with metamaterial as a guiding layer [13]. In 2016, Verma proposed a sensor-chip structure, the performance parameters of which are very high in compared to graphene based and conventional SPR biosensor due high adsorption efficiency of metamaterial film [14]. At the same time, many researchers focused on the strongly localized binding capacity of metamaterial sensing structure and the enhancement effect on the electromagnetic field [15–17]. These features greatly improve the performance of the sensor in detecting extremely low-molecular-weight biomolecules and the interaction of macromolecular material.

The purpose of this paper is to illustrate the unusual performance of a metamaterial based sensor, and to design appropriate structures for biosensing applications. In this study, we analyzed a polarization control method for surface plasmon resonance sensing applications with metamaterials and compared our research with the existing literature. This

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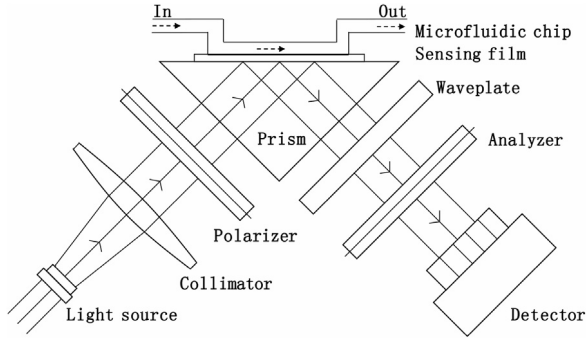


Fig. 1. Schematic of the surface plasmon resonance (SPR) polarization control method.

paper is organized as follows. Section 2 covers theoretical background and essential formulas for investigating sensor properties. Section 3 describes the analysis of the obtained results and comparison with existing literatures. Section 4 presents our conclusions.

## 2. Theory and analysis

### 2.1. Polarization control theory

The polarization control theory [18] was first proposed in 1998, and works by converting the change in polarization to a change in intensity. Polarization control is favorable when compared with other SPR sensors as these systems all have specific drawbacks. Angular modulation [19] is complicated to implement angle scanning system, wavelength modulation [20] is difficult to miniaturize, intensity modulation [21] has a low sensitivity and unsatisfactory anti-interference performance, and phase modulation [22] requires a complicated equipment structure and has a limited dynamic range. The high-sensitivity measurement suitable for high-throughput SPR sensors can be made more easily using a simpler mechanical system and simple structure by using the polarization control method.

In this study, the polarization control method [23] was used to design the SPR sensor. Fig. 1 displays the schematic of this method. Monochromatic light passes through the optical axis after collimation and a polarizer aligned at a certain angle with respect to the horizontal direction produces linearly polarized light with transverse electric (TE) and transverse magnetic (TM) wave components. The light is then obliquely incident on a rectangular prism and is reflected from the prism's face by gold film interface, producing elliptically polarized light. By passing through a quarter-wave plate, because of phase compensation, the elliptically polarized light becomes linearly polarized again. Finally, an analyzer is used to obtain complete extinctions of the linearly polarized light.

The Jones matrix can be used to illustrate the whole process. When light from a light source passes through a polarizer, which forms a polarizing angle  $\psi_{polar}$ , linearly polarized light is obtained:  $E_0 = \begin{pmatrix} \cos \psi_{polar} \\ \sin \psi_{polar} \end{pmatrix}$ . It is then obliquely incident on the rectangular prism and is reflected from the prism's face by the gold film interface, producing elliptically polarized light  $E_1$ . The reflected light can be expressed as:  $E_1 = \begin{pmatrix} \cos \psi_{polar} \cdot r_s \\ \sin \psi_{polar} \cdot r_p \end{pmatrix}$ , where  $r_s$  and  $r_p$  are the reflectivities of the TE and TM waves, respectively. In a three-layer model, they can be calculated from multiple-beam interference as:

$$r_{ik} = \frac{r_{i(i+1)} + r_{(i+1)k} \exp(-i2\delta_{i+1})}{1 + r_{i(i+1)}r_{(i+1)k} \exp(-i2\delta_{i+1})}, \quad (1)$$

where  $r_{ij}$  is the reflectance of different interfaces of the multilayer film, which can be calculated by using Fresnel equations. The refractive index of a metamaterial film is given by Fang et al. [24]  $n = -\sqrt{\epsilon\mu} = n_r + n_i i$ , where  $n_r < 0$  and  $n_i < 0$ ,  $n_r$  and  $n_i$  are parameters that need

to be optimized by the particle swarm PSO (algorithm) optimization. Subscripts  $i$  and  $j$  are equal to 1, 2, and 3 for the prism, gold film, and solution, respectively.  $\delta$  is the phase difference between two adjacent reflections in multiple-beam interferences.

Since  $E_1$  is elliptically polarized light, the azimuth angle  $\psi_{ellip}$  of the long axis can be expressed as:

$$\psi_{ellip} = \frac{1}{2} \cdot \tan^{-1} \left( \frac{2 |\sin \psi_{polar} \cdot r_p| \cdot |\cos \psi_{polar} \cdot r_s| \cos \delta_{ref}}{|\cos \psi_{polar} \cdot r_s|^2 - |\sin \psi_{polar} \cdot r_p|^2} \right), \quad (2)$$

where  $\delta_{ref}$  is the phase difference of the TE and TM wave components of  $E_1$ .

Because the phase difference between the long and short axes of the elliptically polarized light and between the fast and slow axes of the quarter-wave plate is  $\pi/2$ , if the fast axis of the quarter-wave plate rotates to coincide with the long axis of the elliptical polarized light,  $\psi_{waveplate} = \psi_{ellip}$ , the transmission light is linearly polarized and denoted as  $E_2$ . It is expressed as:

$$E_2 = \begin{bmatrix} \cos \psi_{waveplate} & -\sin \psi_{waveplate} \\ \sin \psi_{waveplate} & \cos \psi_{waveplate} \end{bmatrix} \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \times \begin{bmatrix} \cos \psi_{waveplate} & \sin \psi_{waveplate} \\ -\sin \psi_{waveplate} & \cos \psi_{waveplate} \end{bmatrix} \cdot E_1 = \begin{pmatrix} E_{2s} \\ E_{2p} \end{pmatrix}. \quad (3)$$

The light transmission axis of the analyzer is adjusted to the vertical angle of the polarization direction of the polarized light:

$$\psi_{ana} = \tan^{-1} \left( \frac{E_{2p}}{E_{2s}} \right) + \frac{\pi}{2}. \quad (4)$$

This process is called light extinction. We can block a solution (e.g., water) by adjusting both the wave plate and the analyzer with a fixed incident angle and a fixed  $\psi_{polar}$ . When the refractive index of the solution changes, light extinction is no longer complete. Therefore, the changing light intensity caused by changes of refractive index will be detected.

### 2.2. Parameter optimization for PSO for SPR sensor system

Starting with a random initial solution, PSO algorithm is an iterative optimization method [25,26], in which particles follow the best particle to find the optimal set of parameters in the solution space. After each iteration, each particle updates itself by tracking its optimal solution (individual extremum) and the optimal solution currently found by the whole population (global extremum). In this study, we used a three-layer model (gold-metamaterial-gold) as the initial sensing chip, hence seven parameters needed to be optimized, including the incidence angle (range:  $0^\circ$ – $90^\circ$ ), incident polarizing angle (range:  $0^\circ$ – $90^\circ$ ), thickness of the first layer (gold, range: 0–100 nm), thickness of the second layer (metamaterial, range: 0–1000 nm), thickness of the third layer (gold, range: 0–100 nm), real part of the refractive index of the metamaterial (range:  $-2$  to  $0$ ), and the imaginary part of the refractive index of the metamaterial (range:  $0.01$ – $5$ ). These parameters determine the response of the SPR signal. For maximizing sensitivity, the optimal parameters were obtained by the PSO algorithm. The initial parameters of the designed PSO algorithm are shown in Table 1.

In this algorithm, we need to construct an evaluation function that represents the effect of the intensity response with changing refractive index. In other words, it is also a fitness function that describes the results. Instead of using light intensity response, we can define the evaluation index  $F$  of the evaluation function for the response curve as:

$$F = \begin{cases} \frac{\sum_{i=1}^{n-1} |x'_{i+1} - x'_i|}{n-1} \times 10^S & S \geq S_{threshold} \\ 0 & S < S_{threshold} \end{cases}, \quad (5)$$

where  $S$  is the linear correlation coefficient of discrete data  $x'$  (where  $x' = x'(x'_1, x'_2, \dots, x'_{n-1})$ ,  $x'_i = |x'_{i+1} - x'_i|$ ,  $x'_i$  is the light intensity response data), and  $S_{threshold}$  represents the linearity window defined as 0.985.

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