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Optimization methodology for structural multiparameter surface plasmon resonance sensors in different modulation modes based on particle swarm optimization

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ABSTRACT

One of the main challenges in designing plasmonic biosensors is maximizing their sensing performance. This study proposes heuristic algorithms based on surface plasmon resonance-particle swarm optimization (SPR-PSO), which were investigated for the optimization of the sensing performance of structural multiparameter SPR sensors in four modulation modes (phase, intensity, wavelength, and angle). Different fitness functions were designed for different modulation modes that comprised a variety of evaluation indicators (such as sensitivity, figure of merit, full-width-at-half-maximum, electric field intensity, and penetration depth). Four types of available experimental structures representing the various modulation schemes were compared with the corresponding optimized structure by algorithms. The results showed that the introduced algorithms have a considerable efficiency. Furthermore, the algorithms also showed some potential in aiding the parametric design of negative refractive index materials.

1. Introduction

Plasmonic biosensors possess real-time, rapid, and label-free characteristics that allow the detection of the interaction of biological molecules. The basis of the plasmonic sensing mechanism is dependent on the excited charge density oscillation (surface plasmons) propagating along the metal/dielectric interface that can resonate when the wave vector of the incident light satisfies the resonance condition [1–4]. In visible to near-infrared (NIR) wavelengths, the electric fields associated with these oscillations are particularly sensitive to changes in the refractive index of the surrounding medium. Therefore, plasmonic sensors can be used to monitor biological molecules participating in binding events in real time, and they have also been used in important applications in life sciences, food safety, drug screening, and in other areas [5–8].

Surface plasmon resonance (SPR) sensors based on surface plasmon polaritons (SPP) are extensively used as plasmonic biosensors [9,10]. The SPR sensor usually adopts the Kretschmann structure to match the momentum between SPP and the light beam. SPR sensors are usually divided into four modulation methods. These are the angle, wavelength, intensity, and phase modulations. The design of the SPR sensor usually requires the determination of the sensor's structural parameters. These determine the sensitivity of the sensor, the full-width-at-half-maximum (FWHM) value of the resonance curve, the limit of detection (LOD), the electric field strength, and its penetration depth. In addition, the resonance figure of merit (FOM) determined by the sensitivity and the FWHM value can be used as a measure of the detection ability for trace low-molecular-weight biomolecules [11]. However, the inability to detect low-molecular-weight species is also a test bottleneck (< 500 Da) [12]. The lower penetration depth (200–300 nm) of SPR imposes a large limitation when detecting analyte sizes equal to or larger than micrometer-sized organisms, such as cells. In addition, the fabrication process of nanoscale SPR biosensing chips is complicated and costly, and there are specific issues related to this field [13]. Therefore, the design optimization of SPR biosensors is highly meaningful, even though the number of prior investigations has been limited. In order to solve these problems, excellent optimization techniques must be introduced.

In recent years, conducted research on heuristic algorithms has been applied to the numerical optimization of conventional surface plasmon resonance (cSPR) sensor configurations [14–16]. However, these studies only considered the angle-modulated cSPR structure (gold film structure) as a model, which has fewer parameters and lower versatility. At the same time, the fitness function of this model is not well designed, and simply taking the lowest point of the single-mode resonance curve as the basis of its variation limits its applicability. With the development of plasmonic biosensors, novel sensing methods,

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such as long-range surface plasmon resonance (LRSPR) [17], hyperbolic metamaterial (HMM) [18], multilayer surface plasmon waveguide (MSPW) [19], symmetrical optical waveguide (SOW) [20], and others [21,22], has led to the gradual replacement of cSPR. Owing to the presence of the sensor chip with multilayer films, these novel sensors have the characteristics of a multiparametric structure, and a variety of performance (sensitivity of multi-mode resonance, spatial detection capability, and small molecular detection capability). Thus, a more comprehensive and effective intelligent algorithm used to solve the current structural design of plasmonic biosensors, thus yielding optimal parameters and the best sensor performance, has become particularly important.

In this work, the SPR particle swarm optimization (SPR-PSO) algorithm was formulated by combining the Fresnel coefficient matrix method with particle swarm optimization (PSO), so that the optimal SPR sensor structural parameters could be calculated. This study systematically proposes a novel fitness function calculation model corresponding to the four modulation modes listed previously. The fitness function model includes sensitivity, FOM, and penetration depth as three sensor performance indicators. These are normalized and then unified for evaluation. The evaluation model can be adjusted according to the sensor design requirements. The four types of SPR sensing structures in the literature are optimized and analyzed, and performance results that are much superior to the original model structure are obtained. Correlation analyses are also conducted.

2. SPR-PSO theory

2.1. Fresnel coefficient matrix method

SPR involves a multilayer optical thin-film structure. Correspondingly, in this study, the Fresnel matrix method [23] is used to calculate light transmission within the multilayer thin-film structure. When the optical thin film is in the optical field, the electric field vector of each layer is based on the matrix equations, and the electric field distribution in the membrane layer is calculated based on the matrix method.

The optical flow diagram is shown in Fig. 1, where N_i and N_j represent two refractive indices. Considering the optical flow balance on the interface, it is easy to derive the following pair of equations:

$$\begin{aligned} E_i^- &= r_{ij} E_i^+ + t_{ji} E_j^- \\ E_j^+ &= t_{ij} E_i^+ + r_{ji} E_j^-, \end{aligned} \tag{1}$$

where r_{ij} and t_{ij} are the Fresnel reflection and transmission coefficients, respectively. One can also derive the following relations between r_{ij} and t_{ij}:

$$t_{ij} t_{ji} + r_{ij}^2 = 1 \tag{2}$$

$$r_{ij} = -r_{ji} \tag{3}$$

This expression is rewritten as

$$\begin{pmatrix} E_j^+ \\ E_j^- \end{pmatrix} = \frac{t_{ij}}{1 - r_{ij}^2} \begin{pmatrix} 1 & -r_{ij} \\ -r_{ij} & 1 \end{pmatrix} \begin{pmatrix} E_i^+ \\ E_i^- \end{pmatrix}, \tag{4}$$

The inverse matrix can be expressed as

$$\begin{pmatrix} e^{-i\delta_j} & 0 \\ 0 & e^{-i\delta_j} \end{pmatrix}, \tag{5}$$

where δ_j denotes the phase thickness of the light through the film.

According to these ideas, we can obtain the forward and reverse fields of the jth interface in the multilayer film as

$$\begin{aligned} \begin{pmatrix} E_j^+ \\ E_j^- \end{pmatrix} &= \frac{t_1 t_2 \dots t_j}{(1 - r_1^2)(1 - r_2^2)\dots(1 - r_j^2)} \begin{pmatrix} e^{-i\delta_{j-1}} & -r_j e^{i\delta_{j-1}} \\ -r_j e^{-i\delta_{j-1}} & e^{i\delta_{j-1}} \end{pmatrix} \dots \\ &\quad \begin{pmatrix} e^{-i\delta_1} & -r_2 e^{i\delta_1} \\ -r_2 e^{-i\delta_1} & e^{i\delta_1} \end{pmatrix} \begin{pmatrix} 1 & -r_{ij} \\ -r_{ij} & 1 \end{pmatrix} \begin{pmatrix} E_0^+ \\ E_0^- \end{pmatrix} \\ \begin{pmatrix} E_j^+ \\ E_j^- \end{pmatrix} &= \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} E_0^+ \\ E_0^- \end{pmatrix} \end{aligned} \tag{6}$$

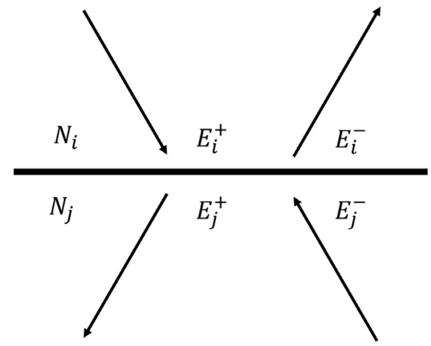

Fig. 1. Optical flow diagram. N_i and N_j represent the two refractive indices. E_i^+ and E_i^- represent the forward electric field and the reverse electric field in N_i, respectively. E_j^+ and E_j^- represent the forward electric field and the reverse electric field in N_j, respectively.

In order to determine the electric field intensity of the jth interface, we need to calculate the amplitude and phase shift of the forward and backward waves.

The physical structure through which light wave propagates shows that E_0^+ and E_j^- are known parameters, and we can express them as

$$\begin{cases} E_j^+ = M_{11} E_0^+ + M_{12} E_0^- \\ E_j^- = M_{21} E_0^+ + M_{22} E_0^-. \end{cases} \tag{7}$$

The values of E_0^+ and E_j^- are determined by solving the matrix equation. Thus, we can obtain the total reflection coefficient of the film structure as:

$$r = E_0^- / E_0^+. \tag{8}$$

The amplitude and phase shift are

$$\left| E_j^+ \right| = \left[(E_{jR}^+)^2 + (E_{jI}^+)^2 \right]^{\frac{1}{2}} \tag{9}$$

$$\delta_j^+ = \tan^{-1}(E_{jR}^+ / E_{jI}^+) \tag{10}$$

where $E_j^+ = E_{jR}^+ + E_{jI}^+$.

The parameters, $\left| E_j^- \right|$ and δ_j^- can be obtained in a similar manner. The electric field intensity E_j is expressed as

$$E_j^2 = \left| E_j^+ \right|^2 + \left| E_j^- \right|^2 + 2 \left| E_j^+ \right| \left| E_j^- \right| \cos(\delta_j^+ + \delta_j^-). \tag{11}$$

By these means, we can obtain the electric field intensity throughout the film.

2.2. Particle swarm optimization

Kennedy and Oberheart first introduced this heuristic algorithm in 1995 [24]. These algorithms are intended to mimic the behavior of natural systems. The algorithm assumes that the particles are searching the solution space for optimal solution points, and the search begins randomly in order to form particles. Thus, the best position of each memory (P_{best}) is explored. Conversely, the total memory of the best position for the population (G_{best}) is obtained by sharing the path of the particle before the state, the best experience of the particles, and the social status of the individual particles in the next path. The particle motion relationship is as follows:

$$\begin{aligned} V_{t+1}^i &= \omega V_t^i + c_1 \cdot rand \cdot (P_{best} - X_t^i) + c_2 \cdot rand \cdot (G_{best} - X_t^i) \\ X_{t+1}^i &= X_t^i + V_{t+1}^i. \end{aligned} \tag{12}$$

V_{t+1}^i is the particle speed at time $t+1$, V_t^i is the particle speed at time t, ω is a weight inertia factor, c_1 is the cognitive critical index, c_2 is the social critical index, $rand$ is a normally distributed random number between zero and one, P_{best} is the best experienced position by the particle, G_{best} is the best experienced position, and X_{t+1}^i and X_t^i are the particle positions at times t and $t+1$.