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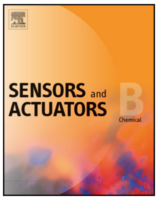

Investigation of surface plasmon resonance phenomena by finite element analysis and Fresnel calculation

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ABSTRACT

In this study, a novel simulated method was developed to provide a graphical and simplistic simulation technique for the purpose of enhancing feasibility of classical surface plasmon resonance (SPR) experiment. Winspall, the software based on the Fresnel equations and the matrix formalism was used to compute the reflectivity of optical multilayer systems. In a simulation study, SPR curves were plotted using Winspall with ultrapure water, 50% ethanol aqueous solvent and pure ethanol as the environmental media. SPR angles of 67.1°, 71.7° and 72.5° were obtained, respectively. These values displayed significant disparity from the experimental data of 62.7°, 65.1° and 65.3° under the same conditions. Finite element analysis (FEA) was then evaluated for its suitability as a better alternative method. By establishing a new Kretchmann SPR model and simulating the S11 parameters, the obtained SPR angles of 62.6°, 65.0° and 65.3° agreed well with the experimental results. Thus FEA method was a more feasible alternative based on our experimental conditions. Hence, an optimal methodology for the theoretical study of SPR detection was developed in this study which contains port boundary conditions, background filed and period boundary conditions. More importantly, this study has established a new avenue of SPR chip applications for portable SPR devices.

1. Introduction

SPR is one of the promising analytical techniques for monitoring biomolecular interaction with good sensitivity [1]. Since the physical phenomenon of SPR was first observed by Wood [2] in 1902, it has been used as a powerful transducer capable of practical applications in sensitive detectors in non-invasive, label-free and time-resolved manner. SPR is a charge-density oscillation. As a surface electromagnetic wave it propagates parallel along the interface of two media with dielectric constants of opposite signs, for instance, a metal and a dielectric [3]. Metals such as silver, gold, copper and aluminium which exhibit free electron behaviour can be used, with silver and gold being more popular. Due to the fact that silver is less stable than gold, the latter is used more widely [4]. For the same reason, gold was employed in this study.

SPR sensor technology has become more useful as a central tool for characterising and quantifying biomolecular interactions. [5] The biological and chemical information can be acquired from a SPR curve which reflects the relationship between angle of incidence and the incidence of reflected light within the resonance reflectance dip. With the development of computer applications, more and more outstanding softwares for application in SPR are available on the market. By the simulation of SPR phenomenon, theoretical data could be obtained to provide an optimal choice for SPR experiment. Some of the common softwares such as Matlab, Winspall, TFCalc, COMSOL and Ansoft HFSS have been used by various researchers [5–8]. Amongst them, Winspall and COMSOL are representative. Winspall uses mathematical analysis based on Fresnel equations and the matrix formalism, and COMSOL requires a simulation model to integral calculate the solved region by a finite element analysis (FEA). For comparative studies, in this work, we employed both Winspall [9] and COMSOL [10].

Most literatures reported numerical analysis concerning nanostructured electromagnetic materials [7,8,11,12], sensor structure [13] and flow pool [14] to improve the design of SPR. Most of these reports lack experimental data to prove the reliability of the simulation results. In addition, there is no literature available in relation to a model based on an actual configuration. In this work, the software Winspall was initially chosen for the simulation study, and ultrapure water, 50% ethanol and pure analytical grade ethanol were selected as environmental media to simulate

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Table 1
Parameters used in simulation.

	Thick (nm)	*n* (refractive index)	*k* (extinction coefficient)
Prism(F1-65)	0	1.616	0
Cr[16]	2	3.07652	3.3498
Au[16]	50	0.16312	3.4624
Water/50%C_2H_5OH/100%C_2H_5OH	0	1.333/1.35605/1.3635	0

the SPR phenomenon. By comparing the mathematical calculations obtained by Winspall with the practical experiment data, a significant disparity was evidenced. Hence, we chose a new approach to establish a simulation model to integral calculate the solved region by COMSOL. Comparing the results obtained by COMSOL with the experimental data show that both analytical feasibility and accuracy were achieved by using this software. The proposed FEA theoretical model produces dissimilar SPR curves and angles in different media. It provides a graphical and simplistic simulation technique which has a great application prospect. A distinct feature of this model is that, it is not limited to a three-layer configuration. A corresponding SPR curve can be plotted and SPR angle calculated if the refractive index and the thickness of a layer were available.

2. Theory and methodology

2.1. The Fresnel equations analysis method

Winspall [9] 3.02 software (Max-Planck-Institute for Polymer Research, Mainz, Germany) was used throughout the simulation. Winspall is a software package for simulation of surface plasmon resonance performance based on the Fresnel's equations [9,15]. By keying in the thickness and refractive index of a layer system and also the dielectric constant which is calculated according to the Fresnel's equation [15], the SPR curve can be plotted. The resonant angle of three media i.e., ultrapure water, 50% ethanol aqueous solvent and 100% analytical grade ethanol were being analysed from the SPR curves in order to determine the integrating degree of SPR. The required parameters used in the simulation are displayed in Table 1. The refractive index of the prism is obtained from the Biosuplar Manual [17]. The parameters of Cr and Au are from the Handbook of Optical Materials [16]. The refractive index parameters of liquid measured at 15 °C were determined from the experimental data by Abbe Refractometer. The wavelength of 670 nm was selected and the prism angle was set as 65° so as to be the same as the experimental prism F1-65. P-polarised light was chosen as the light polarisation.

However, this software was designed for the analysis of smooth surfaces. Hence, using this software to analyse normal SPR sensor chips with their uneven surfaces were found to be inadequate.

2.2. The finite element method

COMSOL Multiphysics [10] was therefore utilised as a simulation platform to calculate resonant angles. The finite element analysis (FEA) is a comprehensive tool for various physics and engineering applications, especially coupled phenomena, or multiphysics. A surface plasmon resonance (SPR) can be considered as the collective oscillation of valence electrons in a solid or liquid stimulated by incident light. The resonance condition is established when the frequency of light photons matches the natural frequency of surface electrons oscillating against the restoring force of positive nuclei. To simply describe the existence and properties of surface plasmons is to take each material for a homogeneous continuum, in which the material's dielectric constant has a complex valued permittivity. For the terms which describe the electronic surface plasmon to exist, the real part of the dielectric constant of the metal must be negative and its magnitude must be greater than that of the dielectric. Fig. 1 shows a layered structure for plasmon excitation.

A layer of gold is sandwiched between two layers i.e., prism and environmental medium (air, water or ethanol) as shown in Fig. 1. If the wave vector of the incident transverse magnetic (TM) wave is k1 and the refracted wave vectors in the next two layers are k2 and k3, then the total TM reflection response of the structure is given as:

$$\Gamma = \frac{\rho_1 + \rho_2\ e^{-2ik_{2x}d}}{1 + \rho_1\rho_2\ e^{-2ik_{2x}d}} \qquad (1)$$

where the TM reflection coefficients ρ_1 and ρ_2 at the interfaces are:

$$\rho_1 = \frac{k_{2y}\varepsilon_1 - k_{1y}\varepsilon_2}{k_{2y}\varepsilon_1 + k_{1y}\varepsilon_2}, \qquad \rho_2 = \frac{k_{3y}\varepsilon_2 - k_{2y}\varepsilon_3}{k_{3y}\varepsilon_2 + k_{2y}\varepsilon_3} \qquad (2)$$

The components k_{1x} and k_{1y} of the incident wave vector k1 are then:

$$k_{1x} = k_0 n_1\ \sin\theta, \qquad k_{1y} = k_0 n_1\ \cos\theta \qquad (3)$$

where $n_1\sqrt{\varepsilon_1}$ is refractive index of incident medium, $k_0 = 2\pi/\lambda_0$ is free-space wavenumber, and λ_0 is free-space wavelength. Because of continuity of the electric field along the interfaces (Snell's law), the transverse components of the wave vector are preserved across the media:

$$k_{1x} = k_{2x} = k_{3x} = k_0 n_1\ \sin\theta \qquad (4)$$

The components $\boldsymbol{k_{2y}}$ and $\boldsymbol{k_{3y}}$ can be calculated from the following relations:

$$k_2^2 = k_0^2\varepsilon_2 = k_{2x}^2 + k_{2y}^2, \qquad k_3^2 = k_0^2\varepsilon_3 = k_{3x}^2 + k_{3y}^2 \qquad (5)$$

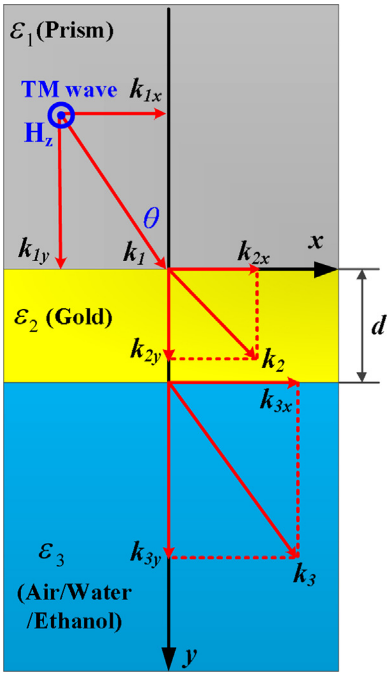

Fig. 1. Surface plasmon excitation structure in a layered structure.