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Numerical Study of Surface Plasmon Resonance in Rough Thin Films under the Kretschmann Configuration

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Abstract. Despite the existence of a developed technology, there are still defects in the manufacture of surfaces for different optical components with optimal performance. In this work we present a numerical analysis of the effects of roughness on surface plasmon resonance (SPR) excitation in a multilayer system under the Kretschmann configuration that is formed by rough conducting and dielectric thin films. To numerically model the optical response of the system, we have used the Integral Equation Method and the Lorentz-Drude model. Furthermore, rough surface profiles are generated by a random Gaussian correlation process that obeys an exponential probability density function, whose parameters are the standard deviation of heights σ and the correlation length δ. In this study we have calculated the reflectance as a function of incidence angle for a normalized Gaussian beam. The results obtained indicate that the SPR angles for the smooth thin films had an angular displacement due to the influence of roughness. Therefore, roughness in surfaces can modify substantially the location of the SPR. These optical properties allow it to have a large number of applications in various fields of science and technology, such as plasmonic sensing.

Keywords: Surface plasmon resonance, Kretschmann configuration, rough thin films, integral equation method.

1 Introduction

The study of multilayer systems are of great interest due to their special optical properties as the absorbance and SPR [3]. The latter, it is based on the confinement of electromagnetic waves on the surface of a metal strongly coupled to collective oscillations of free electrons. The strong confinement of these resonances in the metal surface explains their exceptional sensitivity to changes in the dielectric environment and constitutes the detection mechanism for the development of new technological devices such as solar cells, biosensors or detectors [2, 5]. These surface plasmon oscillations can be excited by electrical or optical stimulation.

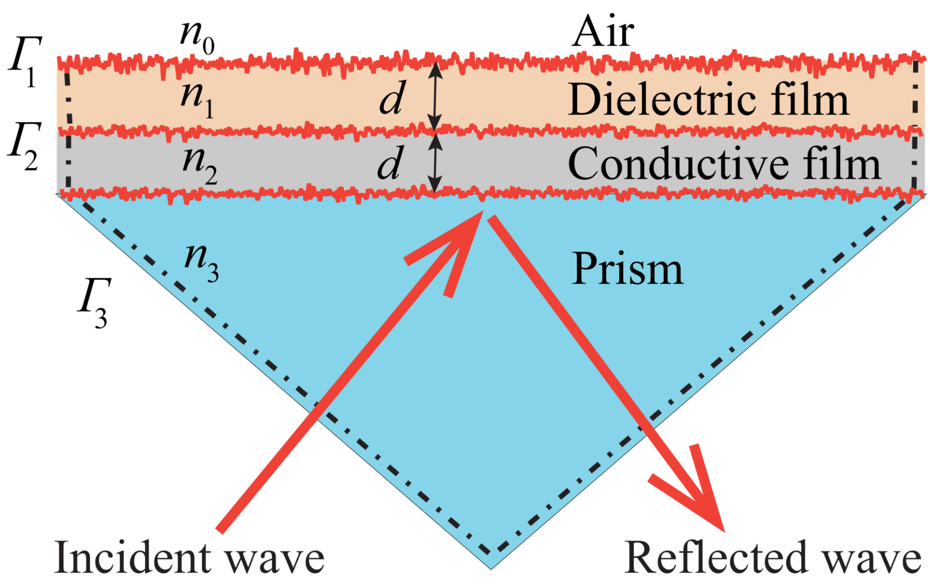

Fig. 1. Diagram of the Kretschmann system formed with rough conductive and dielectric thin films with thicknesses d, characterized by the refractive index n_j for each medium and Γ_j are the contours of the surfaces.

However, excitation cannot be performed by directly incident light on the metal surface because the wave vector of photons is always smaller than that of plasmons. Different techniques have been used to solve this problem, the most important of which is the coupling with a prism called Kretschmann configuration [1]. In this configuration, the metal film evaporates on the prism.

Thus, light illuminates the prism and an evanescent wave penetrates through the metal film, allowing plasmons to be excited on the outer side of the film. This paper is organized as follows. In section 2 we present the system under study and the description of the Integral Equation Method we have used to solve the problem. Section 3 shows the results of the optical response of the system. Finally, in section 4 we present the conclusions of this work.

2 Theoretical Approach

In the present work we will numerically model the SPR in a multilayer system using the Integral Equation Method (IEM) [7, 8] described in this section. The system is shown in Fig. 1. Which is formed of rough conducting and dielectric thin films immersed in an incident medium and a transmission medium with thicknesses d, whose optical properties are given by the refractive index n_j. The rough profile is defined by a random Gaussian correlation process that obeys a negative exponential probability density function, whose parameters are the standard deviation of heights σ and the correlation length δ [4].

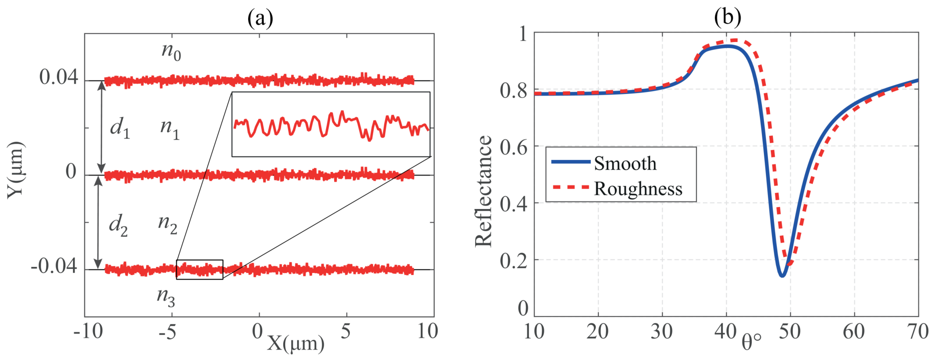

Fig. 2. (a) Profile of the multilayer system under the Kretschmann configuration, which is formed by three interfaces with roughness and four media with refractive indices $n_0 = 1.0$ (air), $n_1 = 1.767$ (Al_2O_3), $n_2 = 0.14316 + i3.7792$ (silver) and $n_3 = 1.723$ (prism) at $\lambda = 629$ nm; layer thicknesses: $d_1 = d_2 = 40$ nm and roughness parameters: $\sigma = 0.001\lambda$ and $\delta = 0.009\lambda$. (b) Reflectances of system formed by rough conductive and dielectric thin films with smooth (solid curve) and rough (dashed curve) surfaces.

2.1 Integral Equation Method

The IEM is based on the numerical solution of the Helmholtz equation which is given by:

$$\nabla^2 \Psi_j(\mathbf{r}) + k_j^2 \Psi_j(\mathbf{r}) = 0, \tag{1}$$

where j indicates the j-th medium, $\mathbf{r} = x\hat{\mathbf{i}} + y\hat{\mathbf{j}}$ is the position vector of the observation point and $\Psi_j(\mathbf{r})$ represents the electric field in the case of TE polarization or the magnetic field in the case of the TM polarization. The magnitude of the wave vector is given by $k_j = n_j(\omega)(\omega/c)$, where the refractive index $n_j(\omega)$ involves material properties and c is the speed of light in vacuum.

To solve equation Ec. (1) let us consider a Green function of the form $G_j(\mathbf{r}, \mathbf{r}') = i\pi H_0^{(1)}(k_j|\mathbf{r} - \mathbf{r}'|)$, where $H_0^{(1)}(z)$ is a Hankel function of the first kind and order zero. Applying the two-dimensional Green second identity to $\Psi_j(\mathbf{r})$ and $G_j(\mathbf{r}, \mathbf{r}')$ to the incident region considered with the prism ($j = 3$) with an incident wave (see Fig. 1), we obtain the scattered field:

$$\Psi(\mathbf{r}) - \Psi_{\text{inc}}(\mathbf{r}) = \frac{1}{4\pi} \int_{\Gamma_3} \left[\frac{G_3(\mathbf{r},\ \mathbf{r}')}{\partial n} \Psi_3(\mathbf{r}) - G_3(\mathbf{r},\ \mathbf{r}') \frac{\partial \Psi_3(\mathbf{r})}{\partial n} \right] ds, \tag{2}$$

where $\Psi_{\text{inc}}(\mathbf{r})$ is the incident field and $G_3(\mathbf{r}, \mathbf{r}')$ is the Green's function in the prism. The source functions $\Psi_3(\mathbf{r})$ y $\partial\Psi_3(\mathbf{r})/\partial n$, represent the values of the electric or magnetic field and its normal derivative evaluated on the Γ_3 contour. For values ($j < 3$) we have:

$$\Psi(\mathbf{r})\Theta(\mathbf{r}) = \frac{1}{4\pi} \int_{\Gamma_j} \left[\frac{G_j(\mathbf{r}, \mathbf{r}')}{\partial n} \Psi_j(\mathbf{r}) - G_j(\mathbf{r},\ \mathbf{r}') \frac{\partial \Psi_j(\mathbf{r})}{\partial n} \right] ds, \tag{3}$$

where $\Theta(\mathbf{r})$ is a function, whose value is one for points in the medium j and zero otherwise.

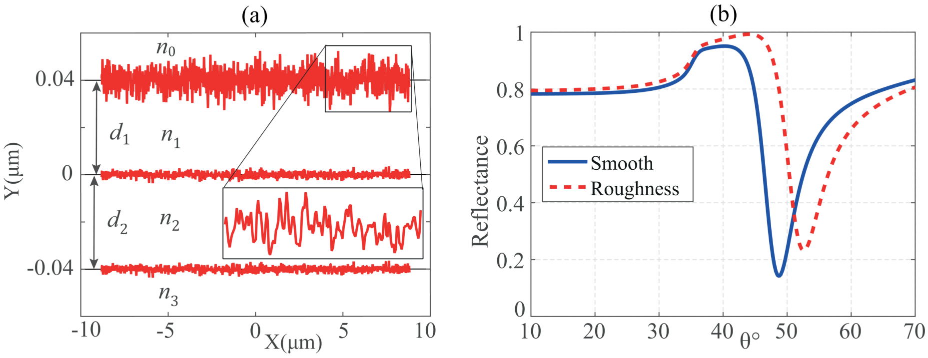

Fig. 3. (a) Profile of the multilayer system under the Kretschmann configuration, which is formed by three interfaces with roughness and four media with $n_0 = 1.0$ (air), $n_1 = 1.767$ (Al_2O_3), $n_2 = 0.14316 + i3.7792$ (silver) and $n_3 = 1.723$ (prism) with roughness parameters: $\sigma_1 = 0.004\lambda$, $\delta_1 = 0.01\lambda$, for the first interfaz and $\sigma_2 = 0.001\lambda$ and $\delta_2 = 0.009\lambda$ for the second and third interfaces. (b) Reflectances of system formed by conductive and dielectric thin films with smooth (solid curve) and rough (dashed curve) surfaces.

Equations (2) and (3) form a system of integro-differential equations with which the total field in the incident and scattering medium can be obtained. To solve them, it is necessary to convert them into matrix equations using a rectangle approximation to evaluate the integrals in small intervals. The details of the discretization of these equations can be consulted in [8, 6]. Once the system of integro-differential equations has been solved, we obtain the values of the source functions with which we can calculate the field at any point. Thus, reflectance can be written as:

$$R(\omega) = \int_{-\pi/2}^{\pi/2} \frac{\partial R}{\partial \theta_s} d\theta_s = \int_{-\pi/2}^{\pi/2} h|A(\theta_s,\, \omega|^2 d\theta_s, \tag{4}$$

where h is a normalization factor that depends on the incident wave and the length of the Γ_3 profile, and $A(\theta_s,\, \omega)$ is the far-field amplitude is given by:

$$A(\theta_s,\, \omega) = \int_{\Gamma_a} \left[-i\frac{\omega}{c}(\mathbf{n}'_a \cdot \hat{\mathbf{r}})\Psi_a(\mathbf{r}') - \frac{\partial \Psi_a(\mathbf{r}')}{\partial n'_a} \right] \times \exp\left(-i\frac{\omega}{c}(\mathbf{r}' \cdot \hat{\mathbf{r}}) \right) ds'. \tag{5}$$

With: $\hat{\mathbf{r}} = (-\cos\theta_s,\, \sin\theta_s)$ and θ_s the angle of scattering.

3 SPR in Rough Thin Films

We analyze the SPR by calculating the reflectance as a function of the angle of incidence for a light beam with $\lambda = 629$ nm. For the excitation of SPR we have used the Kretschmann configuration which is formed by two rough thin films with refractive indices $n_1 = 1.767$ (Al_2O_3) and $n_2 = 0.14316 + i3.7792$ (silver). The mediums surrounding the films are considered with refractive indices $n_0 = 1.0$ (air) y $n_3 = 1.723$ (prism).

In the case of silver, the refractive index was obtained from the Lorentz-Drude model [9]. In Figure 2(a) shows the profile of the multilayer system formed by two rough thin films with thicknesses $d_1 = d_2 = 40$ nm, whose roughness parameters are $\sigma = 0.001\lambda$ and $\delta = 0.009\lambda$. In Fig. 2(b), reflectance of system with rough thin films is shown in comparison with a system consisting of smooth thin films.

Figure 3(a) shows the profile of the multilayer system formed by two rough thin films with thicknesses equal to the previous case. The roughness parameters are $\sigma_1 = 0.004\lambda$, $\delta_1 = 0.01\lambda$, for the first interfaz and $\sigma_2 = 0.001\lambda$ and $\delta_2 = 0.009\lambda$ for the second and third interfaces. In Fig. 3(b) the corresponding reflectances of the system with smooth and rough thin films are shown.

The results obtained in Fig. 2 show that the SPR angle for the smooth case is $\theta = 48.75°$ and for the rough case is $\theta = 49.75°$. In contrast, in Fig. 3, the SPR angle for the rough case is $\theta = 52.5°$ which corresponds to an angular displacement of 3.75 degrees with respect to the smooth case.

4 Conclusions

We have applied the IEM to study the effects of roughness on SPR in Kretschmann configuration. The results obtained show that when considering thin films with small roughnesses, we obtain a slight angular displacement of the minimum value with respect to a system with smooth films. On the other hand, if we consider a combination of films with small and large roughness, we obtain an angular displacement of 3.75 degrees. Also, when considering the two films with large roughness, we obtain a large angular displacement and a higher reflectance with respect to the smooth system.

Therefore, roughness in surfaces can modify substantially the location of the SPR. In general, we have observed that the original position of SPR gradually moves as the roughness parameter δ is increased. Finally, it is worth mentioning that the numerical method used has proven to be reliable for solving problems of this type. This allows this study system to have a large number of applications in various fields of science and technology, such as plasmonic detection.

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