Surface Plasmon Resonance

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Abstract:

Surface plasmons can be generated when specific conditions exist at the interface between two materials. The conditions that determine the formation of plasmons is analyzed and compared to classical analytical expressions. The computational approaches demonstrated here can be used to provide further insight into the behavior of surface plasmons and define conditions under which surface controlled reactions can be characterized.

Keywords: Plasmons, Surface Plasmon Resonance, Surface reaction, Electromagnetic fields.

1. Introduction

Surface plasmons are coherent electron oscillations that exist at the interface between any two materials where the real part of the dielectric function changes sign across the interface. Surface Plasmon Resonance (SPR) can be used to detect molecular adsorption on surfaces and consequently the phenomenon is of significance for technologies ranging from gene assays and DNA sensing, molecular adsorption and desorption on surfaces, surface controlled electrochemical reactions, and nano-scale optical and photonic devices. SPR technology is based on the electromagnetic field component of incident light penetrating tens of nanometers into a surface. The stimulated resonance oscillation of valence electrons reduces the reflected light intensity and produces SPR due to the resonance energy transfer between the evanescent wave and surface plasmons. The resonance conditions are influenced by the type and amount of material adsorbed onto the surface thus allowing characterization of surface related phenomena.

Two commonly used configurations for plasmon excitation exist: the Kretschmann-Raether configuration, in which a thin metal film is sandwiched between a dielectric and air, and the incident wave is from the dielectric side; and the Otto configuration, where an air gap exists between the dielectric and the metal. In both cases, the surface plasmon propagates along the metal/dielectric interface. The Kretschmann-Raether configuration is easier to fabricate but has a fixed dielectric gap that can affect the sensitivity of the measurement.

Full insight into surface plasmon resonance requires quantum mechanics considerations. However, it can be also described in terms of classical electromagnetic theory by considering electromagnetic wave reflection, transmission, and absorption for the multi-layer medium. In fact the excitation of plasmon resonance can only take place if the metal side of the interface is slightly lossy, i.e. when the imaginary part of the metal permittivity is a non-zero negative number. The two configurations typically used for SPR have been analyzed here using COMSOL Multiphysics to define the effect of the SPR on the electromagnetic field.

2. Theory and Model Development

A surface plasmon can be described as the collective oscillation of valence electrons in a solid when stimulated by incident light. The resonance condition is established when the frequency of the light photons matches the natural frequency of surface electrons oscillating against the restoring force of positive nuclei. The simplest way to describe the existence and properties of surface plasmons is to treat each material as a homogeneous continuum, in which the materials' dielectric constant has a complex valued permittivity. For the terms which describe the electronic surface plasmons 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. This condition is met in the IR-visible wavelength region for air/metal and water/metal interfaces - where the real dielectric constant of a metal is negative and that of air or water is positive. Fig. 1 shows a layered structure for plasmon excitation.

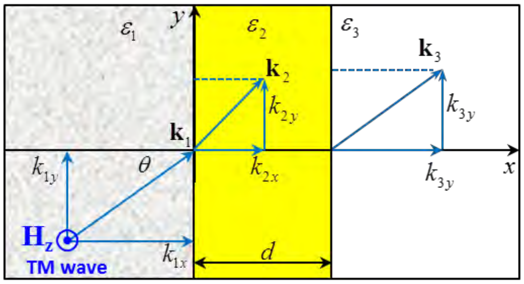

Figure 1: Surface plasmon excitation in a layered structure.

A layer of thickness d and permittivity ε_2 is sandwiched between two layers with permittivity ε_1 and ε_3. If the wave vector of the incident transverse magnetic (TM) wave is $\mathbf{k}_1$ and the refracted wave vectors in the next two layers are $\mathbf{k}_2$ and $\mathbf{k}_3$ then total TM reflection response of the structure is given as [1]:

$$\Gamma = \frac{\rho_1 + \rho_2 e^{-2jk_{2x}d}}{1 + \rho_1 \rho_2 e^{-2jk_{2x}d}} \tag{1}$$

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

$$\rho_1 = \frac{k_{2x}\varepsilon_1 - k_{1x}\varepsilon_2}{k_{2x}\varepsilon_1 + k_{1x}\varepsilon_2}, \quad \rho_2 = \frac{k_{2x}\varepsilon_2 - k_{2x}\varepsilon_3}{k_{2x}\varepsilon_2 + k_{2x}\varepsilon_3} \tag{2}$$

The components k_{1x} and k_{1y} of the incident wavevector $\mathbf{k}_1$ are then:

$$k_{1x} = k_0 n_1 \cos\theta, \quad k_{1y} = k_0 n_1 \sin\theta \tag{3}$$

where $n_1 = \sqrt{\varepsilon_1}$ is refractive index of incident medium, $k_0 = \frac{2\pi}{\lambda_0}$ 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:

$$k_{1y} = k_{2y} = k_{3y} = k_0 n_1 \sin\theta \tag{4}$$

The components k_{2x} and k_{2x} can be calculated from the following relations:

$$\begin{aligned} k_2^2 &= k_0^2 \varepsilon_2 = k_{2x}^2 + k_{2y}^2 \\ k_3^2 &= k_0^2 \varepsilon = k_{3x}^2 + k_{3y3}^2 \end{aligned} \tag{5}$$

Hence,

$$\begin{aligned} k_{2x} &= \sqrt{k_0^2 \varepsilon_2 - k_{1y}^2} \\ k_{3x} &= \sqrt{k_0^2 \varepsilon_3 - k_{1y}^2} \end{aligned} \tag{6}$$

Because expressions in the Eq. 6 can be complex or negative, it is necessary, in complex-waves problems, to get the correct signs of their imaginary parts, such that exponentially decaying evanescent waves are described correctly. This leads to definition of an *"evanescent" square root* as:

$$k_{2x} = \begin{cases} -j\sqrt{\left|k_0^2 \varepsilon_2 - k_{1y}^2\right|}, \\ \sqrt{k_0^2 \varepsilon_2 - k_{1y}^2}, \end{cases} \tag{7}$$

if $\mathrm{Re}\left(k_0^2 \varepsilon_2 - k_{1y}^2\right) < 0$ and $\mathrm{Im}\left(k_0^2 \varepsilon_2 - k_{1y}^2\right) = 0$

and,

$$k_{3x} = \begin{cases} -j\sqrt{\left|k_0^2 \varepsilon_3 - k_{1y}^2\right|}, \\ \sqrt{k_0^2 \varepsilon_3 - k_{1y}^2}, \end{cases} \tag{8}$$

if $\mathrm{Re}\left(k_0^2 \varepsilon_3 - k_{1y}^2\right) < 0$ and $\mathrm{Im}\left(k_0^2 \varepsilon_3 - k_{1y}^2\right) = 0$

This eliminates an exponentially growing field and allows evanescent mode propagation.

The model geometry used here is shown in Fig. 1. The wavelength of the incident light in free-space was taken to be $\lambda_0 = 632$ nm. The model parameters for the Kretschmann-Raether and Otto configurations are summarized in Table 1.

Parameter	K-R	Otto
ε_1	2.25 (Quartz)	2.25 (Quartz)
ε_2	-16-0.5j (Silver)	1 (Air)
d	50 nm	1000 nm
ε_3	1 (Air)	-16-0.5j (Silver)

Table 1: Values of parameters for analysis of Kretschmann-Raether and Otto configurations.

Electromagnetic wave propagation is governed by Maxwell's wave equation in the frequency domain:

$$\nabla \times \frac{1}{\mu_r}(\nabla \times \mathbf{E}) - k_0^2\left(\varepsilon_r - \frac{j\sigma}{\omega\varepsilon_0}\right)\mathbf{E} = 0 \qquad (9)$$

Floquet boundary condition is imposed on the top and bottom surfaces of all layers to enable symmetry of the electric field on the boundaries parallel to the y-z plane. On those boundaries, electric fields differ by a phase shift:

$$E_z\big|_{y=y_2} = E_z\big|_{y=y_2} e^{-j\mathbf{k}_F\cdot(\mathbf{r}_2-\mathbf{r}_1)} \qquad (10)$$

where $\mathbf{r}_2 - \mathbf{r}_1$ is a vector perpendicular to the symmetry boundaries with a magnitude equal to the distance between them. The magnitude of the phase shift depends on the wave number and the incident angle of the plane wave. Since the symmetry boundaries are parallel to the $x-$ axis, only the y component of the wave vector $\mathbf{k}_F$ needs to be defined as given by Eq. (4):

$$\mathbf{k}_F = \{0, k_{Fy}\} = \{0, k_0 n_1 \sin\theta\} \qquad (11)$$

To simulate the incident wave an *Active Port boundary condition* is imposed on the left boundary with a default input power of 1W. The incident TM wave at $x = x_0$ is then described in the form:

$$\mathbf{H}_{TM} = \{0,0,H_z(x_0,y)\}, \quad H_z(x_0,y) \qquad (12)$$

$$\sim e^{-j\mathbf{k}\cdot\mathbf{r}} = e^{-j(k_{1x}x_0 + k_{1y}y)} \sim e^{-jk_{1y}y}$$

Hence, the Port boundary condition at the left incidence plane x=constant is defined as:

$$\mathbf{H}_{TM} = \{0,0,e^{-jk_{1y}y}\} \qquad (13)$$

The propagation constant β normal to the boundary is defined by the x component of the wave vector $\mathbf{k}_1$:

$$\beta = k_{1x} = k_0 n_1^2 \cos\theta \qquad (14)$$

On the right boundary a *Passive Port boundary condition* is imposed to transmit the wave out of the computational domain without reflection. This port condition requires specification of the wave at the boundary and a propagation constant along the outward-facing normal. The TM wave at the boundary is still described by Eq. 13, and the propagation constant at the right boundary is given by Eq. 8:

$$\beta = k_{3x}$$

3. Results

The reflection response of the TM wave versus the incident angle for both the analytical and computational solutions are shown in Figure 3 for the Kretschmann-Raether and Otto configurations; details of the resonance responses are shown in Figure 4. The reflectance is defined as the ratio of the reflected power to the incident power and can be obtained directly from the results of the COMSOL simulation via the scattering parameter S_{11} and from the analytical solutions using Equation 1.

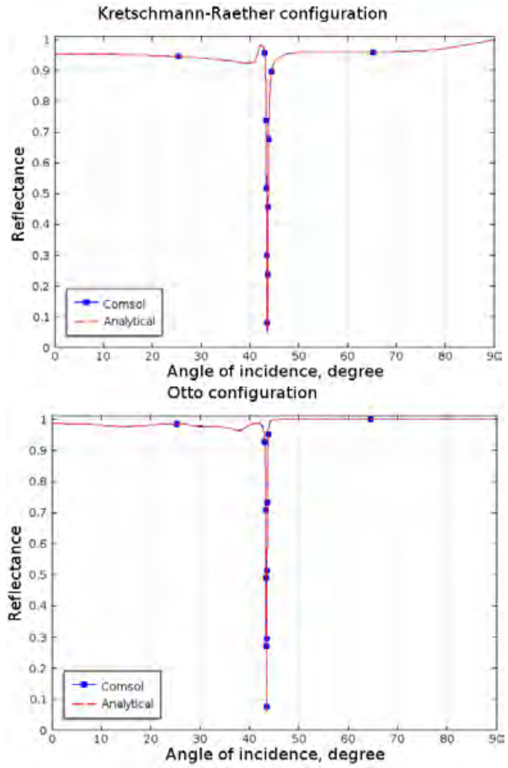

Figure 3: Surface plasmon resonance for Kretschmann-Raether and Otto configurations.

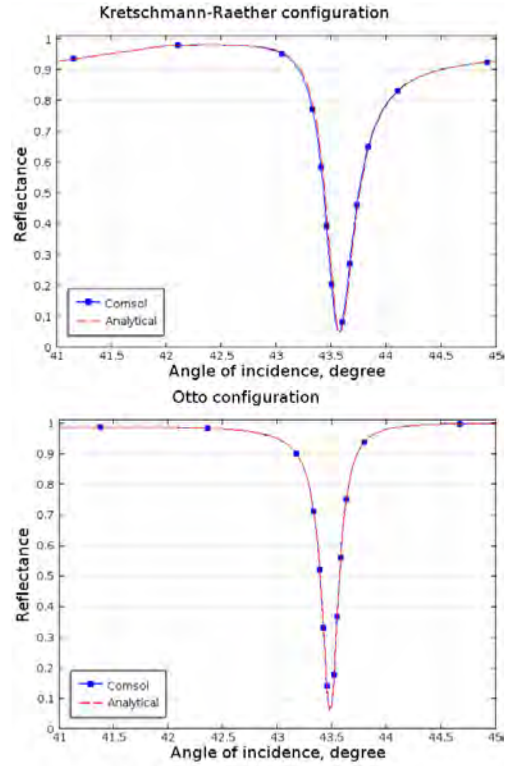

Figure 4: Details of surface plasmon resonance for Kretschmann-Raether and Otto configurations.

The COMSOL simulation and the analytical expressions show good agreement. For the Kretschmann-Raether configuration plasmon resonance occurs at an angle, Θ_{res} ,of 43.58° and for the Otto configuration the angle is 43.49°. Resonance is sharp and its position is sensitive to the dielectric constant of the medium adjacent to metal. This sensitivity is used for the detection of the presence of chemical and biological agents in that medium.

Figure 5 shows magnetic field distributions at resonance. At the resonance angle, a surface plasmon is formed that propagates along the interface. Plots of field distribution along x-coordinate are shown in Figure 6.

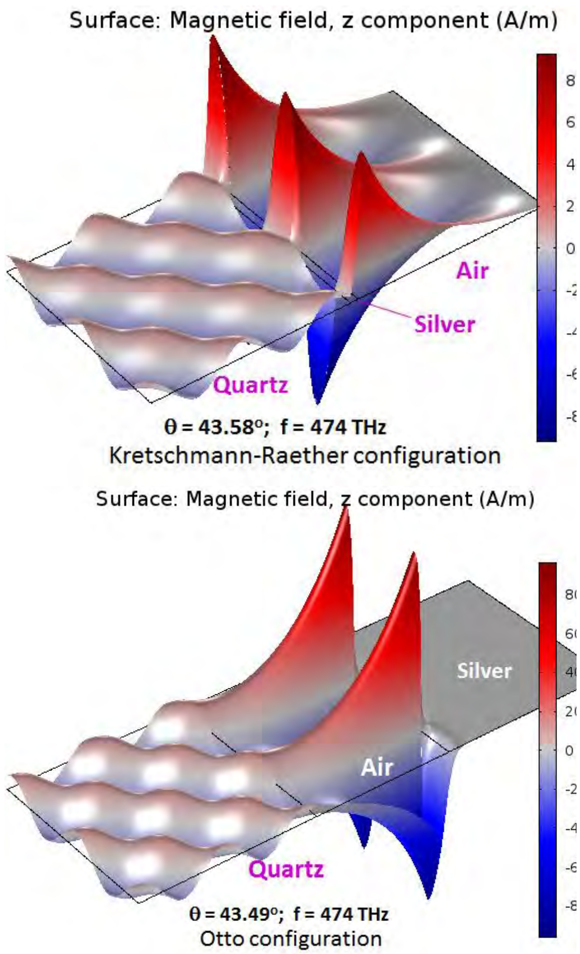

Figure 5: Magnetic field at the resonance angle.

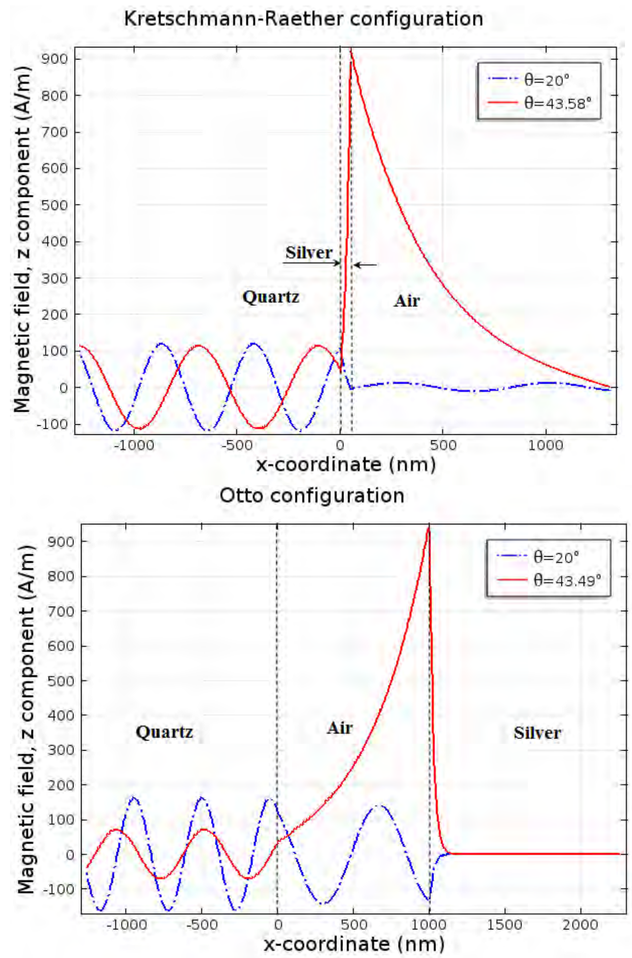

Figure 6: Magnetic field distributions across the media below and at the resonance angle.

To excite plasmon resonance at the metal-air interface the metal material should be lossy. If the imaginary part of metal permittivity is taken to be zero (Figure 7) no plasmon resonance is excited. Under these conditions the wave is purely evanescent in the Kretschmann-Raether configuration below the critical angle and undergoes total internal refraction at, and above, the critical angle. Total internal reflection is observed in Otto configuration for all incidence angles.

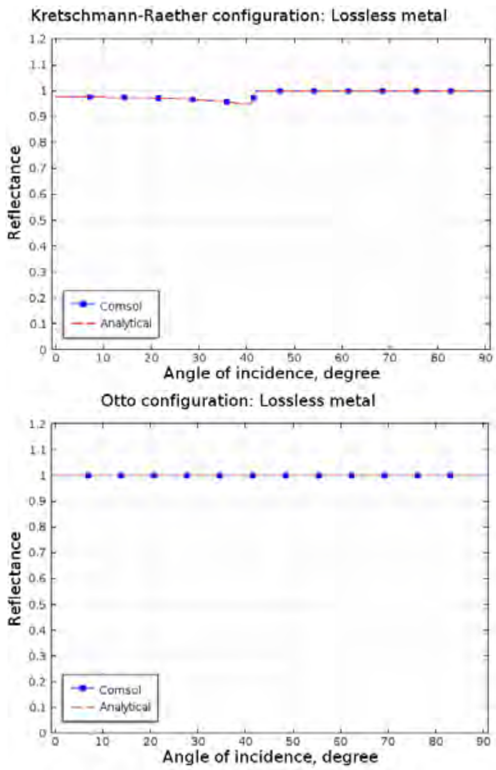

Fig. 7. Absence of resonance when metal is assumed to be lossless.

4. Summary

This paper has demonstrated the analysis of Surface Plasmon Resonance using COMSOL Multiphysics. The two most common configurations for surface plasmon propagation along the metal/dielectric interface have been analyzed. Using the computational approaches demonstrated the effect of different surface and experimental configurations on the SPR response can be defined and thus allow the development of commercial technology for the measurement of surface contaminants and nano-scale photonic devices.

5. References

[1] *Electromagnetic Waves and Antennas*, Sophocles J. Orfanidis, www.ece.rutgers.edu/~orfanidi/ewa/