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Simulations to increase the sensitivity of a prism based plasmonic sensor using MoS_2 - PANI nanocomposite

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Abstract

In this work, we have used prism coupling based plasmonic sensor as a refractive index sensor coated with nanocomposite film over a metal layer. The nanocomposite considered is molybdenum disulphide – polyaniline (MoS_2 - PANI). We did the simulations for prism coupling based plasmonic sensor. In simulations, we studied the variation of sensitivity of the sensor by changing the no. of layers of MoS_2 and observed the variation of sensitivity by changing the volume fraction of MoS_2 in MoS_2 – PANI nanocomposite. For analysis, the effective dielectric constant of nanocomposite is calculated by using Maxwell – Garnett model. It has been found that as we increase the no. of layers of MoS_2, sensitivity increases and as the volume fraction of MoS_2 in MoS_2 – PANI nanocomposite increases, sensitivity further increases more.

Keyword: Surface Plasmon resonance, MoS_2 – PANI nanocomposite etc.

Introduction

Surface plasmon resonance technique has been widely used in recent years for accurate and quick sensing applications. Surface plasmon wave is a p-polarized electromagnetic wave at the metal dielectric interface and it propagates along the interface. When a p-polarized light is incident at metal - dielectric interface and the wave vector of evanescent wave becomes equal to the wave vector of the surface plasmon wave, then maximum absorption of light takes place and at the output end minimum power is obtained. This matching of wave vector is called resonance condition. And this resonance condition is very sensitive and makes this technique widely used for sensing purpose.

For excitation of surface plasmon two methods can be used, one is angular interrogation i.e. varying the angle of incidence and keeping the wavelength of light fixed and other is wavelength interrogation i.e. keeping the angle of incidence fixed and varying the wavelength. Generally, for prism coupling technique, angular interrogation is used.

Basic theory

In prism coupling type, over the base of a high refractive index prism, a thin layer of metal (nearly around 50 nm) is coated and over which a dielectric sensing medium is taken. The evanescent wave generated by the incident light on prism base – metal interface excites the surface plasmon at outer metal – dielectric interface. If we use angular interrogation, then at an angle of incidence resonance condition is achieved and this angle is called resonance angle at which a dip is obtained in reflected light intensity. The resonance condition is expressed as [2]

$$k_{sp} = k_0 \left[\frac{\epsilon_s \epsilon_m}{\epsilon_s + \epsilon_m}\right]^{\frac{1}{2}} = k_{ev} = k_0 \epsilon_p^{\frac{1}{2}} \sin\theta_{res} \quad \text{............ } \mathbf{(1)}$$

Where, k_{sp} is propagation constant of the surface plasmon wave. k_0 represents propagation constant of the incident light. k_{ev} describes propagation constant of the evanescent wave. And ϵ_s, ϵ_m and ϵ_p are dielectric constants of sensing medium, metal and the prism respectively. θ_{res} is the resonance angle.

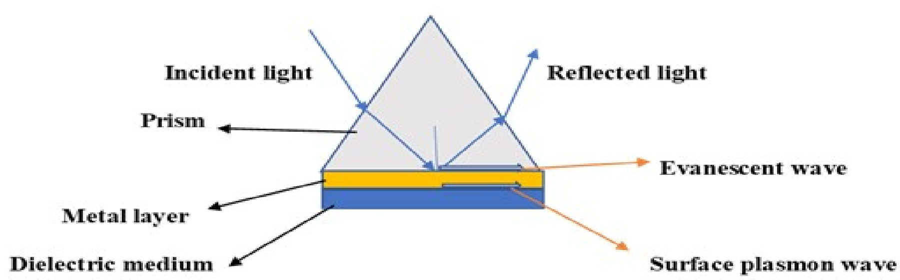

Fig.2.1. Prism coupling

Sensitivity parameters related to the sensing phenomena

If we consider prism based plasmonic sensor with angular interrogation and corresponding to each refractive index of sensing layer n_s and $n_s + \delta n_s$ we get a SPR plot with a dip which is resonance angle as shown in **Fig.2.2**.And due to change in refractive index of sensing layer by δn_s, the shift in resonance angle is δθres is obtained.

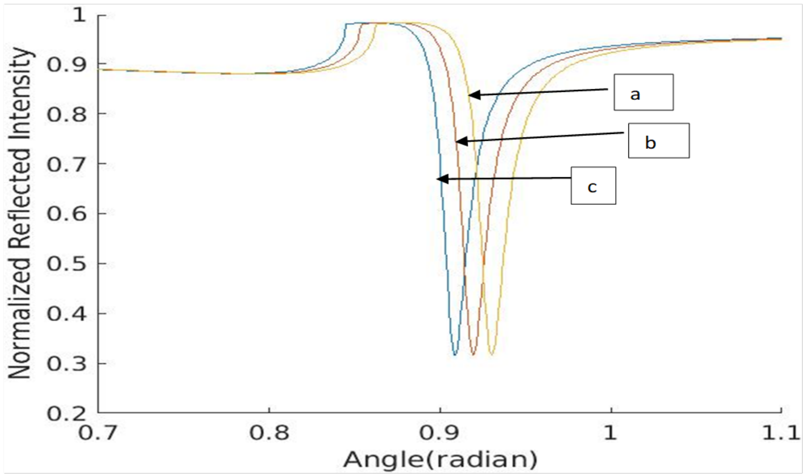

Fig. 2.2. SPR spectra for three different refractive indices of sensing medium

It is defined as the shift in resonance angle with a change in refractive index of sensing layer. Mathematically, it is expressed as[1, 20]

$$S = \frac{\delta\theta res}{\delta ns} \quad \text{.............................} \quad \mathbf{(3)}$$

For the best performance of the sensor sensitivity should be as high as possible.

Theoretical Analysis

For theoretical analysis, we did the simulations to realize a plasmonic sensor in Kretschmann configuration for both prism and fiber based. The purpose of simulations was to analyze different things related to sensor which can be used in fabrication of the sensor and to enhance the sensitivity of the sensor. The simulations were done in MATLAB. For simulations, we used matrix method for multilayer system to obtain the expression for the intensity reflection coefficient (R) for p – polarized incident light beam [4]. We are using this method because it is easy, accurate and without approximations applicable for a system containing any no. of layers. Let us consider multilayer as shown in **Fig.3.1.**where layers is assumed to be stacked along the z axis. An arbitrary medium layer is defined by thickness d_k, refractive index n_k, dielectric constant $\in_k$, permittivity μ_k and angle of incidence of light at first surface is θ_1.

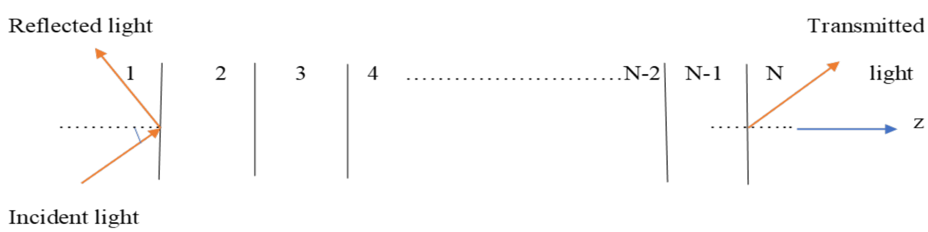

Fig. 3.1. Multilayer model for calculation of reflection coefficient [4]

Tangential fields at the last boundary $z = z_{N-1}$ is related to first boundary $z = z_1 = 0$ by

$$\begin{pmatrix} U_1 \\ V_1 \end{pmatrix} = M \begin{pmatrix} U_{N-1} \\ V_{N-1} \end{pmatrix} \quad \ldots\ldots\ldots\ldots \quad (1)$$

Where, U_1 and V_1 are tangential component of electric and magnetic field respectively at the boundary of first layer. U_{N-1} and V_{N-1} are the corresponding tangential fields at the boundary of Nth layer. And M is the characteristic matrix of the combined structure which is given by

$$M = \prod_{k=2}^{N-1} M_k = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$$

with

$$M_k = \begin{pmatrix} \cos\beta_k & (-i\sin\beta_k)/q_k \\ -iq_k \sin\beta_k & \cos\beta_k \end{pmatrix}$$

Where

$$q_k = \left(\frac{\mu_k}{\in_k}\right)^{\frac{1}{2}} \cos\theta_k = \frac{\left(\in_k - n_1^2 \sin^2\theta_1\right)^{\frac{1}{2}}}{\in_k}$$

and

$$\beta_k = \frac{2\pi}{\lambda} n_k \cos\theta_k \left(z_k - z_{k-1}\right) = \frac{2\pi d_k}{\lambda}\left(\in_k - n_1^2 \sin^2\theta_1\right)^{\frac{1}{2}}$$

Now, for p-polarized incident wave, the amplitude reflection coefficient is given by

$$r_p = \frac{(M_{11} + M_{12}q_N)q_1 - (M_{21} + M_{22}q_N)}{(M_{11} + M_{12}q_N)q_1 + (M_{21} + M_{22}q_N)}$$

Finally, the intensity reflection coefficient for p polarized light is given by

$$R_p = |r_p|^2$$

In prism coupling based simulations, we plot the variation of this normalized reflected intensity with angle of incidence of light in angular interrogation method. And in fiber optic coupling, the normalized transmitted power is calculated for all guiding rays through fiber and generally, we use wavelength interrogation method where we plot the variation in normalized transmitted power with wavelength of incident polychromatic source of light.

Prism coupling based simulations

We can see the prism coupling configuration from **Fig.2.1.** In this case there is a prism, over which there is a metal layer and over the metal layer, there is a sensing layer. For the simulation, we use the multilayer model for the calculation of reflection coefficient and angular interrogation was used. The values have chosen for simulation were [13, 14, 15, 17, 21]

Incident light wavelength = 632.8 nm

Refractive index of the prism =1.7786 (SF11 glass prism)

Metal layer = silver (dielectric constant= -18.281 + i 0.48108

Dielectric constant of MoS_2 = 34.17 + i 9.44

Dielectric constant of polyaniline = 1.71

Dielectric constant of nanocomposite is calculated using Maxwell Garnett model as given equation $\epsilon_{eff} = \epsilon_2 \frac{\epsilon_1 + 2\epsilon_2 + 2f(\epsilon_1 - \epsilon_2)}{\epsilon_1 + 2\epsilon_2 - f(\epsilon_1 - \epsilon_2)}$

Where f is the volume filling factor of first component of the composite?

Monolayer MoS_2 thickness = 0.65 nm

Polyaniline thickness = 6 nm

In this case, silver layer is taken over the prism and the sensing medium is over the silver layer. Here due to many layers we use the matrix method for multilayer system as discussed above. The first task was to find the optimized thickness. The optimized thickness is considered that thickness at which Sensitivity is high and dip of SPR plot is more i.e. there is a proper coupling of evanescent wave with surface plasmon wave. In order to achieve the optimized thickness, we changed the thickness of silver layer to 30nm, 40nm and 50nm at the refractive index of sensing layer 1.33,1.34,1.35 as shown in **Fig.3.2.**At each thickness, we calculated the sensitivity.

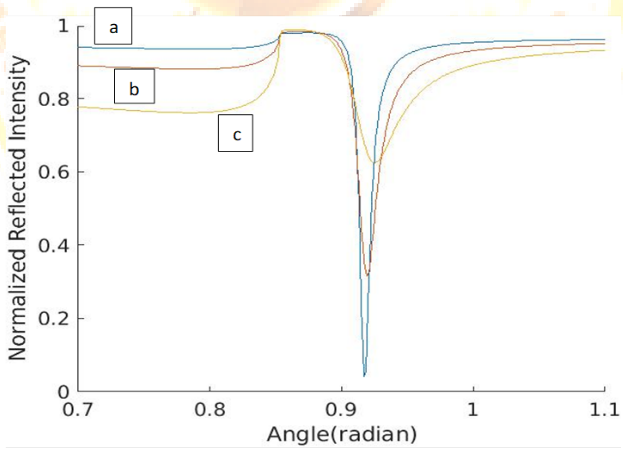

Fig.3.2. SPR plot of prism/ Ag at different thickness at (a) 50nm (b) 40 nm (c) 30 nm

Table 3.1. Variation of sensitivity with thickness of Ag layer

Thickness of Ag layer (nm)	Sensitivity (degree /RIU)
30	63.02
40	63.02
50	57.29

From **Fig.3.2**. and **Table 3.1.,** we can see that the sensitivity at 40 nm thickness of Ag layer is high as well as dip of SPR plot is also good. Hence 40 nm thickness is optimized thickness of silver layer.

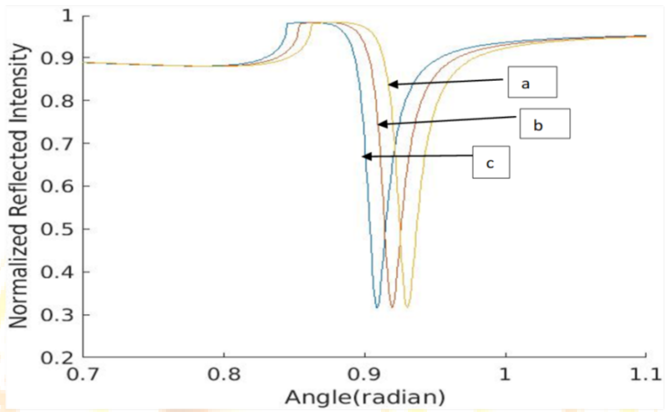

Fig. 3.3. SPR plot of prism / Ag (40 nm) at different refractive index of sensing layer (a) 1.35 (b) 1.34 (c) 1.33

In **Fig.3.3.** SPR plot is shown at different refractive index of sensing layer where silver layer thickness is taken 40 nm.

Now, we took a layer of MoS_2 over the silver layer and then changed the no. of layers of MoS_2 as shown in **Fig.3.4.**At each layer we calculated the sensitivity and observed the variation in sensitivity with no. of layers of MoS_2.

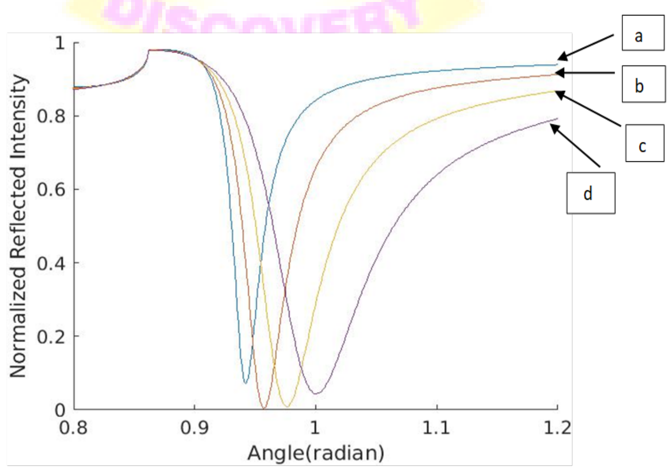

Fig. 3.4. SPR plot of prism / Ag (40 nm) / MoS_2 at different layer (a) 1 layer (b) 2 layer (c) 3 layer(d) 4 layer

Table 3.2. Variation of sensitivity with no. of layers of MoS_2

No. of layers of MoS_2	Sensitivity(degree / RIU)
1	63.02
2	68.75
3	74.48
4	74.48
5	85.94

From **Fig.3.4.** and **Table 3.2.**, we can see that the sensitivity increases as the no. of layers of MoS_2 increases but SPR curve broadens and hence detection accuracy decreases. It means at the 3 layersof MoS_2 (thickness = 1.95 nm) both sensitivity and detection accuracy are good which can be taken as the optimized thickness of MoS_2.

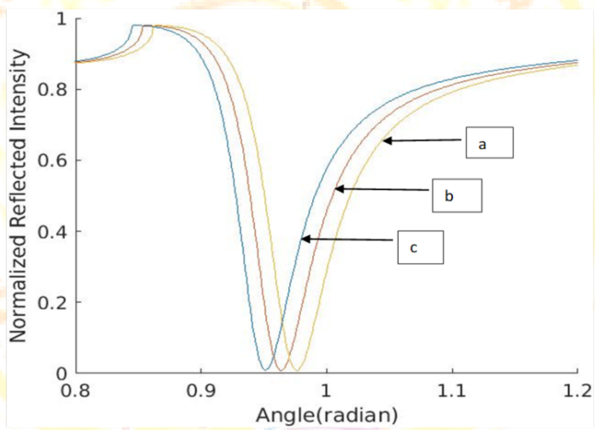

Fig. 3.5. SPR plot of prism / Ag (40nm) / MoS_2 (1.95 nm) at different refractive index of sensing layer (a) 1.35 (b) 1.34 (c) 1.33

In **Fig.3.5.**SPR plot is shown at different refractive index of sensing layer where thickness of silver and MoS_2layer is taken 40 nm and 1.95 nm respectively.

Now, we took a layer of MoS_2 – PANI nanocomposite of thickness 7.95 nm over the silver layer and changed the f values of the nanocomposite and we observed the variation of sensitivity with the f values of the MoS_2 – PANI nanocomposite.

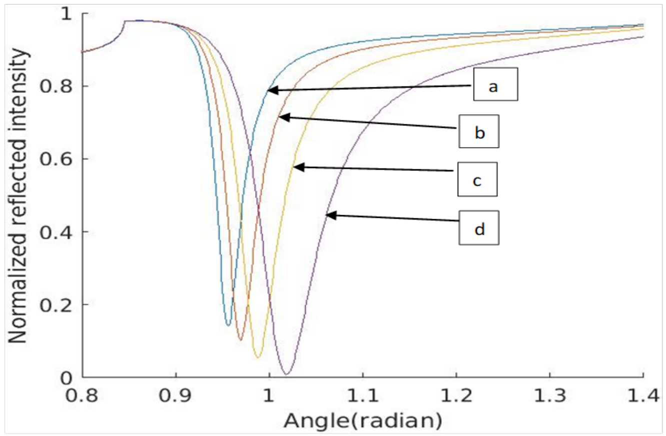

Fig. 3.6. SPR plot of prism / Ag(40 nm) / MoS_2 – PANI nanocomposite(7.95 nm) at different f values (a) 0.45 (b) 0.55 (c) 0.65 (d) 0.75

Table 3.3. Variation of Sensitivity with f values

f values of MoS_2 – PANI nanocomposite	Sensitivity (degree / RIU)
0.45	68.75
0.55	74.48
0.65	80.21
0.75	85.94

From **Fig.3.6.** and **Table 3.3.**, we can see that the sensitivity increases as the f value of the MoS2 – PANI nanocomposite increases and SPR curve broadens but not so poor.

Simulation results and discussion

In prism coupling based simulations, we have following results

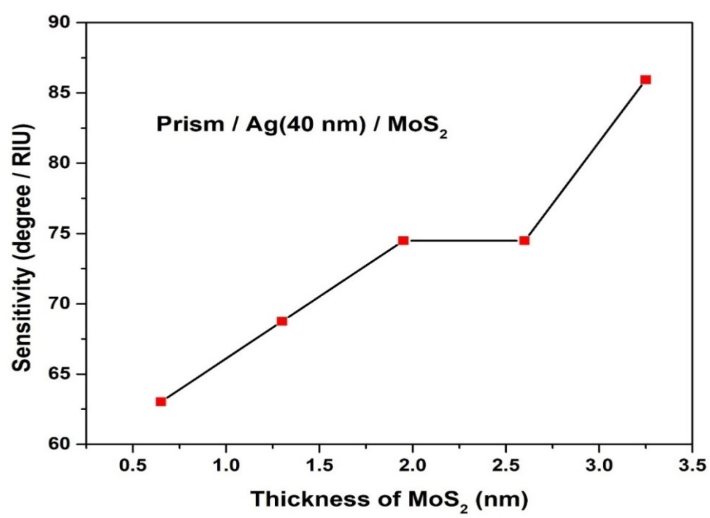

Fig.4.1. Variation of sensitivity with MoS_2 layer thickness (or no. of layers)

From above **Fig. 4.1.** we can see that as the thickness of MoS_2 (or no. of layers of MoS_2) increases, the sensitivity increases. It means if we want to fabricate a plasmonic sensor whereMoS_2material is used then we can use this property of MoS_2 to achive high sensitivity requirement of the plasmonic sensor.

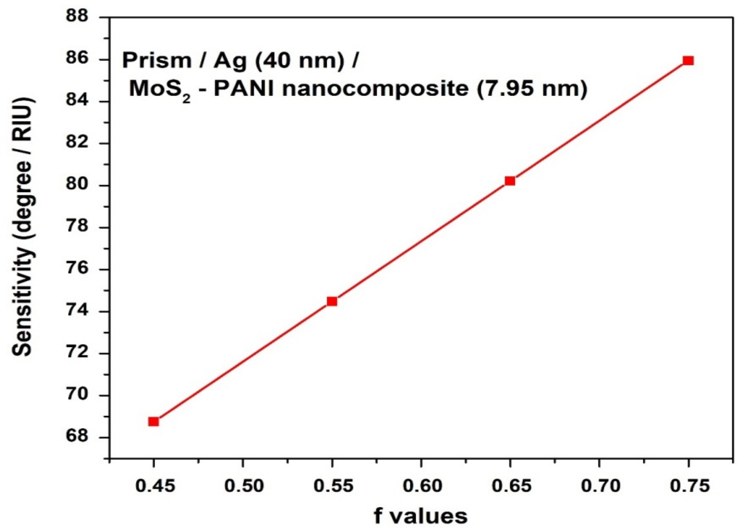

Fig4.2. Variation of sensitivity with f values of MoS_2 – PANI nanocomposite

From above **Fig4.2** we can see that as the f values of the MoS_2 - PANI nanocomposite increases, sensitivity increases. It means if we want to fabricate a plasmonic sensor where MoS_2– PANI nanocomposite is used then we should take as possible as the large volume fraction of MoS_2 in compositeto achive high sensitivity requirement of the plasmonic sensor.

Conclusion

In summary, we have analyzed a prism based plasmonic sensor based on surface plasmon resonance coated with a MoS_2 – PANI nanocomposite as a refractive index sensor. For simulation, the effective dielectric constant was calculated using Maxwell - Garnett model. Then the variation the sensitivity with the no. of layers of MoS_2 was studied for prism coupling based simulations. The result was as we increased the no. of layers of MoS_2, the sensitivity also increased. Then we studied the variation of sensitivity with the f values of the MoS_2 – PANI nanocomposite and we observed that as f values (volume filling factor of first component which is MoS_2 in this case) increased, the sensitivity also increased.

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