Theoretical analysis of a high-performance surface plasmon resonance biosensor using BlueP/WS₂ over a Cu-Pt bimetallic layer

Myilsamy Muthumanicam[1], Micheal Cecil Lordwin Prabhakar[1], Alagu Vibisha[2], Ponnan Suresh[1], Zbigniew Jaroszewicz[3] Karupiya Balasundaram Rajesh[2*]

[1]*Dept. of ECE, Vel Tech Rangarajan R & D Inst. of Science and Technol., Chennai– 600025, Tamilnadu, India,*
[2] *Department of Physics, Chikkanna Government Arts College, Tirupur -641602, Tamil Nadu, India,*
[3]*Łukasiewicz Research Network - Tele & Radio Research Institute, ul. Ratuszowa 11, 03-450 Warsaw, Poland.*

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Abstract—The present theoretical study exhibits the possibility of achieving an incredibly highly sensitive surface plasmon resonance-based biosensor comprising a Cu-Pt bimetallic layer and a BlueP/WS_2 hybrid nanostructure for an angular interrogation method. Based on the Transfer matrix method, the thickness of Cu and Pt and the number of BlueP/WS_2 layers are optimized to obtain the best possible sensitivity and FOM. A well-optimized Cu-Pt-BlueP/WS_2 hybrid structure generates sensitivity as high as 502°/RIU with an FOM of 128.7RIU^{-1}. Such a sensor is handy for detecting biomolecules.

In recent years, surface plasmon resonance (SPR) has been found to be a potential sensing technique owing to its advantages, such as real-time measurement, stable performance, high sensitivity, and accurate detection [1]. Typically, the SPR sensing technique considerably utilizes the Kretschmann configuration, which has the advantages of having a metal film directly coated over the prism, applying a monochromatic light source, and achieving a high signal-to-noise ratio [2]. Gold (Au) and silver (Ag) are primarily chosen as the ideal SPR metals for SPR sensors [3]. On the other hand, Copper (Cu) is cost-effective and produces a much sharper resonance curve compared to Au and Ag. However, Cu is chemically reactive, which affects the SPR sensor stability, and hence needs a protective layer to tackle this issue [4, 5]. Sharma *et al*. demonstrated that a thin platinum (Pt) can be utilized as a protective layer when deposited over Cu to prevent Cu from oxidizing and enhance the sensor sensitivity [6]. Platinum is chemically more stable, inert, highly reflecting, and possesses a high melting point [7]. The BlueP/TMDCs are widely used two-dimensional (2D) heterostructure nanomaterials in biosensors owing to their large charge transfer, high energy bandgap, high mobility, good work function, and optical absorption [8]. Liu *et al.* reported that adding a BlueP/WS_2 layer over a Nickel layer significantly improved the sensor sensitivity to 270°/RIU [9]. Shivangani *et al*. reported that the SPR sensor with an added BlueP/WS_2 layer as an outer layer improved the sensitivity up to 374◦/RIU and acted as a protecting layer with enhanced absorption of biomolecules [10]. This theoretical work suggested a modified Kretschmann configuration that employs a CaF_2 prism, Cu-Pt bimetal, and BlueP/WS_2.

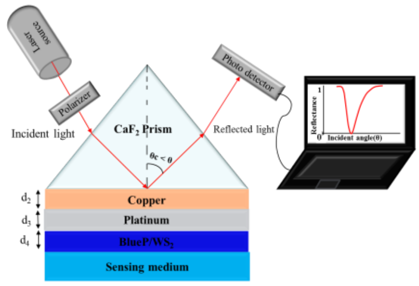

Fig. 1. Schematic diagram for the SPR biosensor with the proposed Cu-Pt- BlueP/WS_2 structure.

The schematic design of the suggested SPR biosensor developed as a modified Kretschmann configuration is illustrated in Fig. 1. This proposed biosensor is a five-layer structure made of Cu-Pt-BlueP/WS_2. We considered a 633nm wavelength p-polarized laser as the source. The refractive index of a CaF_2 prism is given as n_1= 1.4329 [10]. The dielectric constant of metals involved are calculated using the Drude-Lorentz model $\varepsilon_m(\lambda) = \varepsilon_{mr} + \varepsilon_{mi} = 1 - (\lambda^2\lambda_c / \lambda_p^2(\lambda_c + i\lambda))$, where the collision wavelength (λ_c) and plasma wavelength (λ_p) for Cu and Pt [5, 7] are shown in Table 1. The monolayer BlueP/WS2 (L) thickness is 0.75nm, and the refractive index is 2.48+0.17i [10]. The sensing medium is located in the fifth layer with a refractive index of n_s = 1.33 (water).

Metal	λ_c (m)	λ_p (m)	Ref.
Cu	4.0852×10^{-5}	1.3617×10^{-7}	[5]
Pt	1.795×10^{-5}	2.415×10^{-7}	[7]

Table 1

We obtain the reflected light intensity (reflectance) by using N-layer matrix method [11]. In the proposed model, there are five layers (N=5). The reflection coefficient (r_p) of the p-polarized incident light through the multilayer structure will be:

$$r_p = \frac{(M_{11} + M_{12}q_N)q_1 - (M_{21} + M_{22}q_N)}{(M_{11} + M_{12}q_N)q_1 + (M_{21} + M_{22}q_N)}. \quad (1)$$

Reflectance (R_p) for p-polarized light is:

$$R_p = |r_p|^2. \quad (2)$$

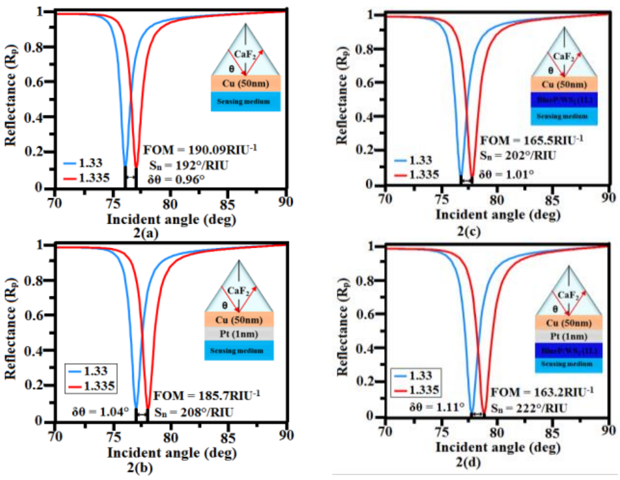

Fig. 2. (a-d) Reflectance as a function of the incident angle at δn_s = 0.005 for the different structures: (a) Cu = 50nm (b) Cu= 50nm & Pt = 1nm (c) Cu= 50nm & BlueP/WS_2 (L = 1) (d) Cu= 50nm, Pt = 1nm, & BlueP/WS_2 (L = 1).

The two most important SPR sensor performance parameters are sensitivity and figure of merit (FOM), which are defined as [9]: (i) Sensitivity (S_n) is the ratio between the switching of the resonance angle ($\delta\theta_{SPR}$) and the sensing medium refractive index variation (δn_s) and is given as:

$$S_n = \frac{\delta\theta_{SPR}}{\delta n_s}(\text{deg/ RIU}). \quad (3)$$

(ii) The figure of merit is defined as the ratio between the sensitivity and FWHM:

$$FOM = \frac{S}{FWHM}(\text{RIU}^{-1}). \quad (4)$$

Figure 2a shows the reflectance curve for the SPR sensor with a fixed thickness of the Cu layer at 50nm. We consider that adding the biomolecules to the sensing medium changes the refractive index of the sensing medium to 0.005 (i.e., δn = 0.005). The resonance curve for the above configuration is plotted, based on Eq. (2), and the corresponding shift in resonance angle $\delta\theta$ is measured as 0.96° with sensitivity and FOM calculated as 192°/RIU and 190.09RIU^{-1} respectively. However, for the protection purpose, a 1nm Pt layer added on a 50nm Cu layer shows the resonance curves as shown in Fig. 2b. It is clearly noted that by using a Pt layer, the resonance angle shifting is larger (1.04°) with a corresponding increase in the sensitivity as 208°/RIU and a decrease in FOM as185.7RIU^{-1}. This clearly shows that including a Pt layer exhibits high sensitivity due to Pt having a higher real part of the dielectric constant [3]. In the next phase of study, a 2D-layer is further added to increase the biomolecules absorption efficiency and investigate the effect of BlueP/WS2 on the sensitivity of the proposed biosensor. In Figure 2c, we noted that adding a monolayer of BlueP/WS_2 without a Pt layer enhanced a shift in the resonance angle $\delta\theta$ as 1.01° and calculated sensitivity (S_n) and FOM as 202°/RIU and 165.5RIU^{-1} respectively. Figure 2d shows that by simultaneously adding Pt and BlueP/WS_2 on the copper layer, the shift in the resonance angle is further increased as $\delta\theta$ = 1.11° and the corresponding sensitivity improved as S_n = 222°/RIU with FOM as 163.2RIU^{-1}. Hence, it can be clearly observed that the proposed sensor composed of the Pt and monolayer of BlueP/WS_2 exhibits maximum sensitivity.

d_{Pt} (nm)	d_{Pt} (nm)	No of BlueP/WS_2	R_{min} at n_s		FWHM (deg) at n_s		$\delta\theta_{SPR}$ (deg)	S_n (°/RIU)	FOM (RIU^{-1})
			1.33	1.335	1.33	1.335			
0	50	1	0.038	0.032	1.22	1.3	1.01	202	165.5
1	50	1	0.015	0.01	1.36	1.47	1.11	222	163.2
2	50	1	0.002	0.003	1.54	1.68	1.23	246	159.7
3	50	1	0.001	0.006	1.76	1.96	1.42	284	161.3
4	50	1	0.016	0.041	2.06	2.38	1.7	340	165.04
5	46	1	0.002	0.033	2.77	3.32	2.07	414	149.4
6	40	1	0.014	0.015	3.9	4.49	2.51	502	128.7

Table 2

We further analyzed the Pt layer effects on the proposed biosensor's sensitivity, which is shown in Fig. 3. We plotted sensitivity, R_{min}, and FWHM versus the varied thickness of Cu (d_{Cu}) for a fixed Pt thickness (d_{Pt}) from 1nm to 6nm. It is noted that by increasing the Pt layer thickness, the sensitivity and FWHM value increase. R_{min} close to zero is essential for a sensor for coupling the maximum energy of incident light with the surface Plasmon. The maximum sensitivity obtained at all near-zero R_{min} for a particular Cu layer thickness for the fixed thickness of Pt is listed in Table 2. Here it is noted that the best result obtained at such a condition is a 6nm Pt layer inserted between the 40nm copper and the 1-layer of BlueP/WS_2.

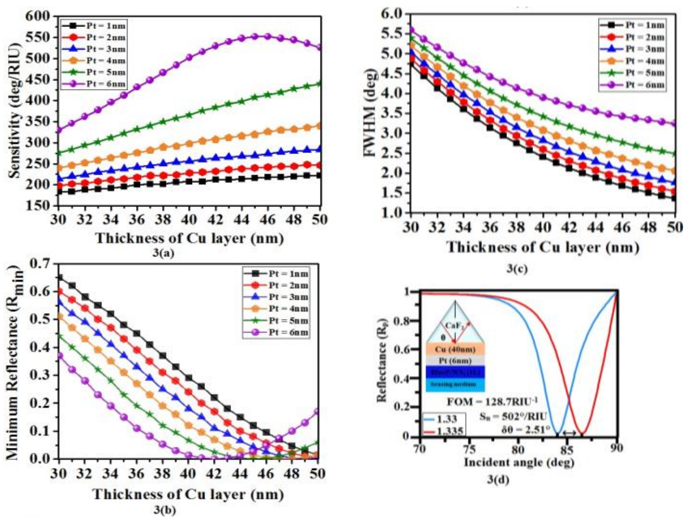

Fig. 3. (a-c) Sensitivity, R_{min}, FWHM versus the Cu layer thickness varied from 30nm to 50nm. (d) Reflectance plot for Cu= 40nm, Pt = 6nm, and BlueP/WS_2 (L = 1).

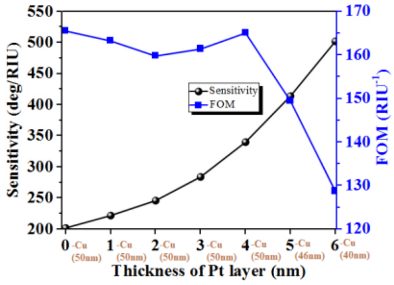

Fig. 4. Sensitivity and FOM vs. thickness of Pt layer for the optimized Cu layer.

Figure 4 shows that with increasing Pt layer thickness, sensitivity increases but FOM decreases. However, a 6nm Pt layer exhibits high sensitivity (502°/RIU) and high FOM (128.7RIU^{-1}). The results obtained are compared with similar SPR sensors proposed recently and shown in Table 3. So the proposed biosensor provides high sensitivity and high resolution as well.

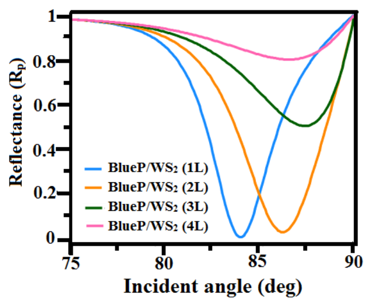

Fig. 5 Reflectance vs. angle of incidence for various numbers of BlueP/WS_2 layers with fixed Cu= 40nm & Pt = 6nm at n_s = 1.33.

λ nm	SPR sensor structure	S_n (°/RIU)	FOM (RIU^{-1})	Ref
633	CaF_2-Zno-Au-BlueP/MoS_2	228	56.21	[8]
633	SF10-Ni-BlueP/MoS_2	270	-	[9]
633	CaF_2-Cu-BlueP/MoS_2	272.9	-	[13]
633	CaF_2-Ag-Si-BlueP/MoS_2	282	55.12	[14]
633	BK7-Cu-Ni-BP-$Ti_3C_2T_x$	304.47	57.85	[15]
633	FK51A-Ag-$BaTiO_3$-BlueP/MoS_2	347.82	60.521	[16]
633	CaF_2-Ag-Al_2O_3-Ni- BlueP/WS_2	374	-	[10]
633	CaF_2-Cu-Fe_2O_3-antimonene	398	-	[17]
633	CaF_2-Cu(40nm)-Pt(6nm)-BlueP/WS_2 (1L)	502	128.7	proposed

Table 3.

We also analyzed the effect of the number of BlueP/WS_2 layers, as depicted in Fig. 5. It is obvious that with an increase in the number of BlueP/WS_2, the resonance angle shift is increased with an increase in FWHM of the resonance curve. Such an increase in FWHM is due to the fact that the SP wave propagation velocity in 2D materials slows down, which causes damping. As the FWHM is linearly proportional to damping, a broadening SPR curve occurs and makes it challenging to identify the resonance angle and a decrease in the FOM [12]. So, the number of BlueP/WS_2 layers must be optimized rather than randomly increased to achieve the best sensitivity of a biosensor. Hence on the basis of the above optimization here we have concluded that the proposed biosensor comprised of (40nm) Cu, (6nm) Pt, and BlueP/WS_2 (L = 1) exhibits extremely high sensitivity as 502°/RIU and FOM as 128.7RIU^{-1}.

In conclusion, this numerical study investigated an ultrahigh-sensitive SPR sensor consisting of a Cu-Pt-BlueP/WS_2 hybrid structure for the detection of biomolecules. We observed that sensitivity improved greatly when adding a Pt layer on the Cu layer. Here, BlueP/WS_2 plays an important role in increasing sensitivity due to its high optical absorption. We also optimized the thickness of Cu-Pt layers, and number of BlueP/WS_2 layers to achieve high sensing performance. The proposed SPR sensor with a well optimized hybrid configuration consisting of Cu-Pt- BlueP/WS_2 exhibiting sensitivity as high as 502°/RIU and FOM as high as 128.7RIU^{-1} is expected to be very useful for biomolecular detection.

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