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بررسی تأثیرساختارناهمگون واندروالسیِ فسفرن آبی- دی کالکوژنید فلزات واسط (MoS_2,WS_2,$MoSe_2$,WSe_2) بر افزایش حساسیت زیست حسگرتشدید پلاسمون سطحی

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چکیده– دراین مقاله تأثیر ساختار ناهمگون واندروالسیِ فسفرن آبی-دی کالکوژنید فلزات واسط (دی سلنید تنگستن،دی سولفید تنگستن،دی سلنید مولیبدن،دی سولفید مولیبدن) باضخامت های مختلف درساختار زیست حسگر تشدید پلاسمون سطحی(SPR) در نرم افزار لومریکال شبیه سازی و بررسی شده است. ساختار پیشنهادی براساس ساختار کرشمن می باشد که درآن از منشورباجنس BK_7، لایه ی طلای ۳۰نانومتری ولایه فسفرن آبی/دی کالکوژنید فلزات واسط استفاده شده است.مشاهده می شود که حداقل مقدار بازتاب برای ۶لایه فسفرن آبی/دی سلینید تنگستن و لایه ۳۰نانومتری طلا رخ می دهد که حساسیت در این ساختار برای $\Delta n=$ ۰/ ۰۰۹ برابر ۱۵۱/۸۸ °/RIU ودقت تشخیص نیزبرابر ۰/۰۸۷ است.

کلیدواژه– بازتاب، تشدید پلاسمون سطحی، حساسیت، زیست حسگر ،ساختار ناهمگون واندروالسی فسفرن آبی/ دی کالکوژنید فلزات واسط.

Investigating the Effect of Blue Phosphorene-MX_2 (MoS_2,WS_2, $MoSe_2$,WSe_2) Vander Waals Heterostructure on the Enhancements Sensitivity of an SPR-Biosensor

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Abstract- In this paper, the effect of Blue Phosphorene - transition metal dichalcogenides (Blue P-TMDs) vander Waals (vdW) Heterostructure layer with different thickness on the structure of surface plasmon resonance (SPR) biosensor in a Lumerical software environment is simulated and investigated. The main structure is based on the structure of Kretschmann and the use of the BK_7 prism, the gold(Au) layer, and the end layer of Blue P-TMDs or Blue P-MX_2(MoS_2, $MoSe_2$,WS_2,WSe_2). It was observed that the minimum reflectance of ۰،۰۰۲ is achieved for Au(۳۰nm) / Blue P-WSe_2(٦-Layer). The combination also yields a sensitivity of ۱۵۱،۸۸ °/RIU for Δn = ۰،۰۰۹ with a great detection accuracy of ۰،۰۸۷.

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Keywords: Biosensor, Blue P-TMDs vdW heterostructure, Reflectance Surface Plasmon Resonance, Sensitivity.

١. Introduction

Surface plasmon resonance sensors are one of the types of optical sensors which measure various biologics and chemical parameters based on the interaction between the sample medium and the sensor surface.[١], [٣] To excite surface plasmons at the metal-dielectric interface, the electrons of the metal conduction band must be able to resonance with input light on the surface at a given wavelength.[٢]

In surface plasmon resonance based biosensors, gold or silver is generally coated directly onto the prism to separate the sensor medium from the prism. Biomolecules have a low capacity to interact with gold, which reduces the sensitivity of the sensor.To resolve this problem, in recent studies of biosensor structure, one or more layers of graphene have been used because of the high surface-volume ratio, high electrical mobility and stability of the atomic structure.[٢] However, it does not act as a semiconductor due to insufficient of bandgap in its electronic structure.[٤] This deficiency prevents its use in numerous applications, including optoelectronics. Transitional metal dichalcogenides (TMDs), another important component of the ٢D material family,have also aroused scientists' interest.The most common TMDs are molybdenum disulfide ($MoS_٢$), Tungsten disulfide ($WS_٢$), Molybdenum diselenide ($MoSe_٢$) and Tungsten diselenide ($WSe_٢$) They have a perceptible band gap, allowing the conversion of electrons into light photons and resulting in extraordinary on/off ratios. [٥]

Today, other ٢D materials such as Black phosphorene(BlackP) and Blue phosphorene (BlueP) are being investigated. However, BlackP and BlueP are easily degraded in ambient air.[٦] BlueP has the same hexagonal crystalline structure and lattice parameter as TMDs, such as $MoS_٢$, $MoSe_٢$, $WS_٢$ and $WSe_٢$. To avoid the BlueP of external agents, a combination of ٢D materials with BlueP is developed, resulting in the possibility of vander Waals (vdW) heterostructure. Moreover, this heterostructure plays an important role in the improvement of the optical and electronic stability properties of materials compared to their ٢D shapes.[٧]

In the present article, a structure consisting of different layers of Blue Phosphorene-TMDs ($MoS_٢$, $MoSe_٢$, $WS_٢$, $Wse_٢$) vander Waals(vdW) Heterostructure on an Au layer has been proposed. The structure formed as an SPR biosensor at ٦٣٢ nm incident light. The various structures were then simulated in the Lumerical environment and modifications of the refractive index were investigated and compared.

٢. The Proposed SPR-Biosensor Structure

In this paper, we use the ٤-layer Krishmann structure, including the prism, gold(Au) layer, Blue P-TMDs vdW heterostructure, and sample environment, respectively. The physical properties of the different materials used for the simulation are presented in Table I.

Table I. Refractive index and thickness different layers.

Layer	Refractive Index	Thickness
Prism[٨]	١,٥١٥	-------
Au[٨]	٠,١٨٥+٣,٤٢٣i	٣٠nm
BP-$MoS_٢$[٩]	٢,٨١+٠,٣٢i	٠,٧٥nm
BP-$WS_٢$[٩]	٢,٤٨+٠,١٧i	٠,٧٥nm
BP-$MoSe_٢$[٩]	٢,٧٧+٠,٣٥i	٠,٧٨nm
BP-$WSe_٢$[٩]	٣,٠٠+١,١٤i	٠,٧٨nm

Important parameters in the surface plasmon resonance sensor that reflect the performance of this sensor include: Sensitivity(S); Indicates the rate of change of sensor output to the measured characteristic changes, expressed as follows.

$$S = \frac{\Delta \theta_{SPR}}{\Delta n} \qquad (١)$$

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Detection accuracy(D.A)Indicates the proximity of the measured characteristic to its true value, and It is mentioned in relation ۲.

$$D.A = \frac{\Delta\theta_{SPR}}{FWHM} \qquad (۲)$$

The quality factor ; It is expressed by Equation ۳. [۱۰]

$$Q = \frac{S}{FWHM} \qquad (۳)$$

۳. Results and Discussion

The aims of this article is to investigate a new detection configuration with using layers of Blue P-TMDs($MoS_۲$,$WS_۲$,$MoSe_۲$,$WSe_۲$) on a thin layer of gold to improve the capacity of the light absorption of the SPR-biosensor and to further enhance its sensitivity.As shown in Fig.۱, we first examine the structure with the Au/Blue P-TMDs(۱L) sensitive layer and compare it with the results of the gold monolayer at the top of the prism.

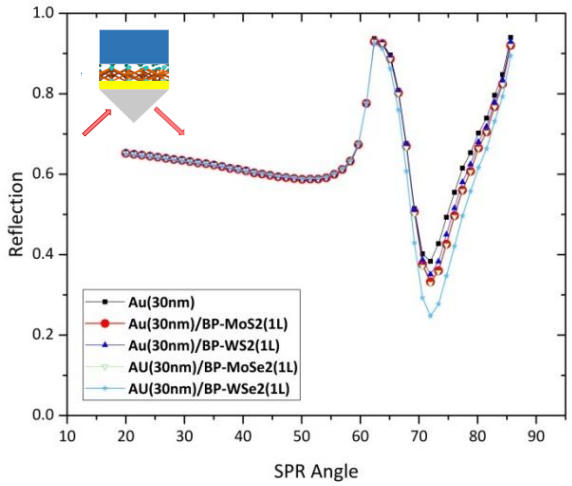


Fig. ۱: Illustration of the SPR-biosensor structure

As can be seen in Fig. ۱, the minimum reflectance(R_{min}) in the structure with the Au layer and the thickness of ۳۰ nm is ۰,۳۸۳ and by adding an additional monolayer of Blue P - TMDs($MoS_۲$,$WS_۲$,$MoSe_۲$,$WSe_۲$) on Au a ~۳۵٪ reduction in R_{min} occures in ۰,۲٤۷ and an approximate difference in SPR angle is $\Delta\theta \approx$ ۰°. This is achieved in the best conditions for theBlue P – $WSe_۲$ layer.By retaining the Au layer thickness at ۳۰nm, the impact of additional layer of Blue P-$WSe_۲$ on the minimum reflectance of the Au(۳۰nm)/Blue P -$WSe_۲$ configuration was also investigated and compared. As shown in Fig. ۲, when the thickness of Blue P/ $WSe_۲$ layer grows the lowest reflectance approaches ۰,۰۰۲ for Au(۳۰nm)/ Blue P-$WSe_۲$(٦L). Table II, lists the minimum reflectances corresponding to the angles of occurance for the setup simulation at different thickness of Blue P/$WSe_۲$ layers in Au۳۰ / Blue P-$WSe_۲$ configurations in n = ۱,۳۳ enviornment.

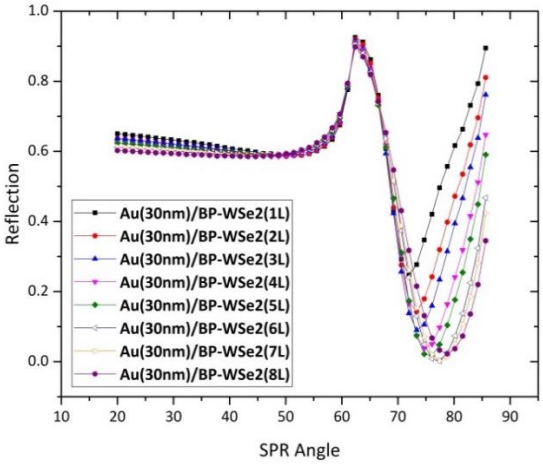


Fig. ۲: The reflection spectra for different thickness of Blue P-$WSe_۲$ layers in Au(۳۰nm)/ Blue P-$WSe_۲$

Table II. Resonance angle (θ°) and *Rmin* values for different thickness of Blue P/$WSe_۲$ layers in Au۳۰ / Blue P-$WSe_۲$ configurations in n = ۱,۳۳ enviornment.

Layer number of Blue P/$WSe_۲$	Resonance Angle(θ°)	Minimum Reflectance(R_{min})
۱	۷۱,۹۵	۰,۲٤۷
۲	۷۳,۳۲	۰,۱٤۲
۳	۷۳,۳۲	۰,۰۹۰
٤	۷٤,٦۹	۰,۰۳۸
٥	۷٦,۰٦	۰,۰۱۷
٦	۷۷,٤۲	۰,۰۰۲۰
۷	۷۷,٤۲	۰,۰۰۲۸
۸	۷۸,۷۹	۰,۰۲۲

From the results of Fig. ۱ and ۲ we can see that the minimum reflectance happens at ۰,۰۰۲. This means that the combination Au(۳۰nm)/BP-$WSe_۲$(٦L) is the most optimal structure among the available configurations. By modifiying the

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medium to n = ۱,۳۳۹,the sensor's sensitivity and the spectral response of the Au(۳۰nm)/BP-WSe_2(٦L) structure are investigated. Fig. ۳ indicates the response of the spectral reflection to various environments. Sensitivity, can now be determined using the above mentioned Eq. (۱) and the details of Fig. ۳ for replies to n = ۱,۳۳۰ and n = ۱,۳۳۹.which are listed in Table III based on Fig. ۳ information. The results of another investigation into Au(۳۰nm)/ G(۲L) are also presented for comparison. [۱۱]

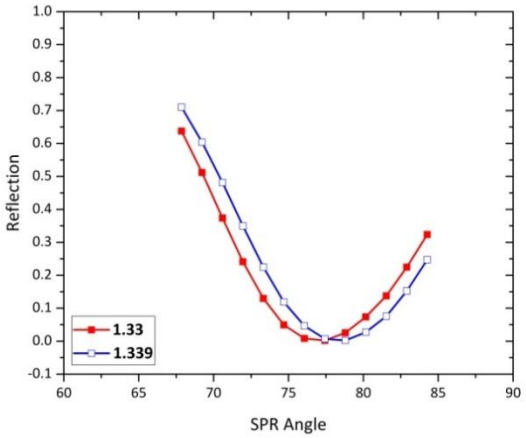


Fig.۳: The reflection spectra for Au(۳۰nm)/BP-WSe_2(٦L) configuration at watery (n = ۱,۳۳۰) and analyte (n = ۱,۳۳۹) representing .

Table III. The sensitivity (*S*), detection accuracy (*DA*), and quality (*Q*) of the proposed Au(۳۰nm)/BP-WSe_2(٦L) SPR-biosensor vurses work in [۲۸]for n = ۱,۳۳۹ medium.

SPR-Biosensor Configuration	Au(۳۰nm)/BP-WSe_2(٦L)	Au(۳۰nm)/ G(۲L)
FWHM	۱٥,۷	۲۲,۰٦
Δθ SPR	۱,۳٦۷	٦,۲٥
***S* (°/RUI)**	۱٥۱,۸۸	۸۹,۲۹
DA	۰,۰۸۷	۰,۲۹
Q	۹,٦۷	٤,۲٦
ref	This work	[۱۱]

٤. Conclusion

In this work, the effect of different Au(۳۰)/BP-TMDs(MoS_2,WS_2,$MoSe_2$,WSe_2) combinations and the number of their flakes on the spectral response of an SPR biosensor was investigated and presented. Moreover, a comparison was made between the structure of layer and the medium. The results indicate that the BP-WSe_2(٦L) on Au(۳۰nm) has the highest sensitivity, which is ۱٥۱,۸۸°/RIU. The results also show that increasing the thickness of layers in the output has a direct effect on the sensor's efficiency and improves sensor performance.

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