

RESEARCH PAPER

The Effect of Different Metal Layers on the Absorption of One-Dimensional Structures Including WS₂ Monolayer and Spacer Layer

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ARTICLE INFO

Article History:

Received 19 September 2022

Accepted 25 December 2022

Published 01 January 2023

Keywords:

Absorption

Metal layer

Optoelectronic

Spacer

Transition metal dichalcogenides

WS₂ monolayer

ABSTRACT

Due to their optical characteristics, nanomaterials like WS₂ monolayer are of huge importance in photonic sensors and photovoltaic elements. Here, we propose designing a multi-layer structure based on metal and spacer layer to enhance light absorption of WS₂ monolayer. The transfer matrix method is employed to study the optical characteristics of the structure. The maximum increase of absorption is observed when the spacer is inserted between metal and WS₂ monolayer. Optimizing the thicknesses of the spacer and metal layer, which is chosen among Au, Ag, Cu, and Al, increases the light absorption of WS₂ monolayer at a specific wavelength. The increase in the absorption of all of the four metals at the wavelength of 619 nm is almost equal (About 62%) but the amount of absorption of Au and Cu is higher than that of other metals in the visible range and absorption above 80% is observed only in these two metals. The results of this study provide new prospects for preparing high-performance optoelectronic devices

How to cite this article

Ansari N., Mohebbi E., Ghomashi T. The Effect of Different Metal Layers on the Absorption of One-Dimensional Structures Including WS₂ Monolayer and Spacer Layer. J Nanostruct, 2023; 13(1):184-192. DOI: 10.22052/JNS.2023.01.020

INTRODUCTION

Owing to their exceptional optical properties, two-dimensional materials like transition metal dichalcogenides (TMDC) have gained significant importance in photonic sensors and photovoltaic elements in the recent years. TMDCs, the most important member of which is Tungsten disulfide (WS₂) monolayer, have a direct band gap and high absorption in the visible wavelength range [1]. WS₂ monolayer has three direct band gaps in the visible range [2]. WS₂ monolayer is used in ultrasensitive photodetectors because of their narrow band of optical absorption centered at 619nm. The light absorption of WS₂ monolayer

should increase to extend its applications to optoelectronic devices. Thus far, several physical methods have been proposed to enhance the interaction of WS₂ monolayer with light. In these methods, the absorption of light has increased in a wide wavelength range or at a specific wavelength. Multilayer structures including spacer [3], plasmonic metal nanostructures as a substrate [4], thin layers [5] or gratings [6], defective photonic crystals [7], and defective quasi photonic crystals [8] have been proposed to achieve higher amounts of absorption at a specific wavelength.

Placing WS₂ next to the metal nanoparticles

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to increase the absorption of the structure have received much attention in the fundamental studies as well as designing optoelectronic devices [9, 10]. In particular, metals can be utilized to enhance light absorption due to their intrinsic plasmonic resonances or reflected light [11, 12]. The type of the metal and its work function are likely to affect the absorption of the structure. Most studies have designed two-dimensional structures with nanoparticles, air holes or a metal layer with a grating [13-15]. However, due to their easy design and construction as well as their lower costs, one-dimensional structures are more desirable options for achieving higher amounts of absorption.

Looking for higher amounts of absorption, in the present work we investigate the effect of different metal layers, i.e., Au, Ag, Cu, and Al, on the absorption of one-dimensional structures including WS₂ monolayer and spacer layer. The presence and different thickness of the metal layer and spacer on the absorption of the structure, specifically at wavelengths of 619 and 432 nm, and the effect of experimental errors have been studied. Hence, our results are likely to open up a new avenue of improving the light-matter interaction in WS₂ monolayer for being utilized in optoelectronic applications.

MATERIALS AND METHODS

A schematic of the proposed structure to enhance the absorption, air/WS₂/spacer/metal/substrate, is shown in Fig. 1, in which WS₂ monolayer lies between the air and the spacer and a thin layer of metal has been deposited onto the substrate. SiO₂ was chosen as the substrate and spacer layers and Au, Ag, Cu, or Al were selected as the thin layer metal.

The light is obliquely incident on the structure from the air with an angle of incidence θ_{in} ; the absorption spectra were calculated by employing the transfer matrix method [3]. This method requires the real (n) and the imaginary (k) refractive index and the thickness of the constituted layers. The thickness of WS₂ monolayer is 0.618 nm and the thicknesses of the spacer and metal layers are represented by d_s and d_{Metal} , respectively. The dependence of the complex refractive index on the wavelength for SiO₂, Au, Ag, Cu, Al, and WS₂ monolayer in the visible wavelength range were extracted from the Ref. [16-19, 2]. Fig. 2a shows n and k of WS₂ monolayer. Moreover, transmission, reflection, and absorption spectra of suspended WS₂ are plotted in Fig. 2b. The absorption spectra show three peaks with the amount of absorption of 19%, 8%, and 17% located at the wavelengths of 434, 517, and 619 nm, respectively. The

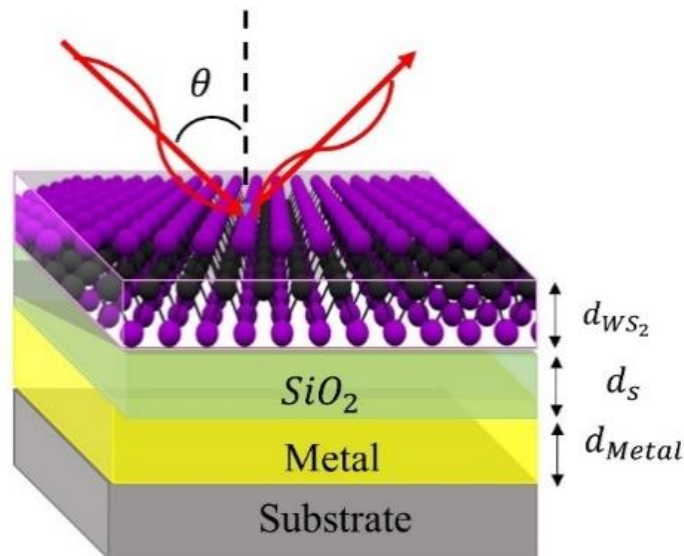


Fig. 1. Schematic of the structure, air/WS₂/spacer/metal/ substrate. The thickness of the spacer, WS₂ monolayer and metal layers present d_s , d_{WS_2} and d_{Metal} respectively.

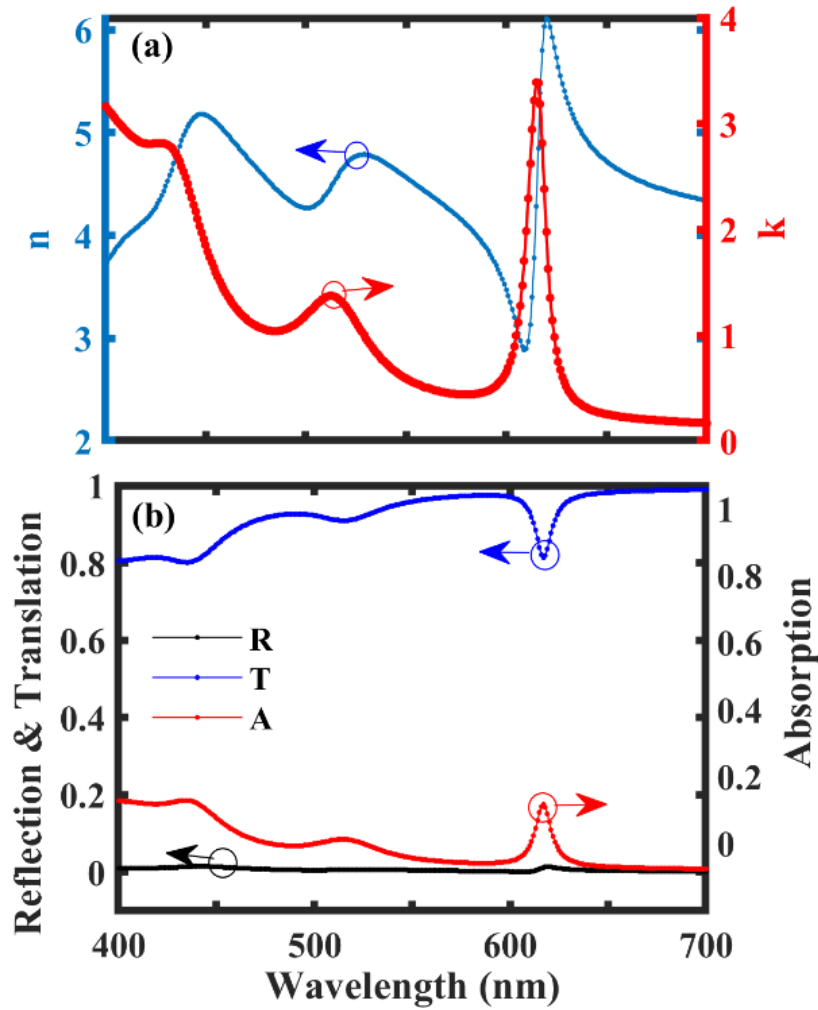


Fig. 2. (a) The Real (n) and the imaginary (k) refractive index of the WS₂ monolayer. (b) Transmission, reflection, and absorption spectra for suspended WS₂.

sharpest peak of WS₂ monolayer is found at 619 nm. A comparison between panels a and b in Fig. 2 indicates that the absorption peaks and k correspond to each other.

Further, n and k of the Au, Ag, Cu, and Al layer are displayed in Fig. 3. The imaginary part of the refractive index in Al is larger than that in other metals. With increasing the wavelength, refractive index k of the Au, Ag, Cu, and Al layers rises from 500 nm, 420 nm, 600 nm and 400 nm, respectively.

RESULTS AND DISCUSSION

Absorption spectra illustrated in Fig. 4 show various thicknesses of Au, Ag, Cu, and Al. By increasing the thickness of metal layer from a

given number (40nm for d_{Au} and d_{Ag} , 20nm for d_{Cu} and 5 nm for d_{Al}) the amount of absorption does not exceed a specific value. A metal layer was placed between WS₂ monolayer and the substrate to investigate the effects of the metal layer on the absorption; the thickness of the metal layer is a crucial parameter in increasing the absorption. As displayed in Fig. 5, the absorption spectrum was plotted as a function of the thickness of the metal layer and the wavelength of air/WS₂/metal /substrate structure. According to the Fig, compared to the absorption of the suspended WS₂, the absorption of the structure increases slightly. For example, as shown in Fig. 5b, the absorption of $d_{Au} = 0$ at $\lambda=619$ nm is 12% and the maximum value

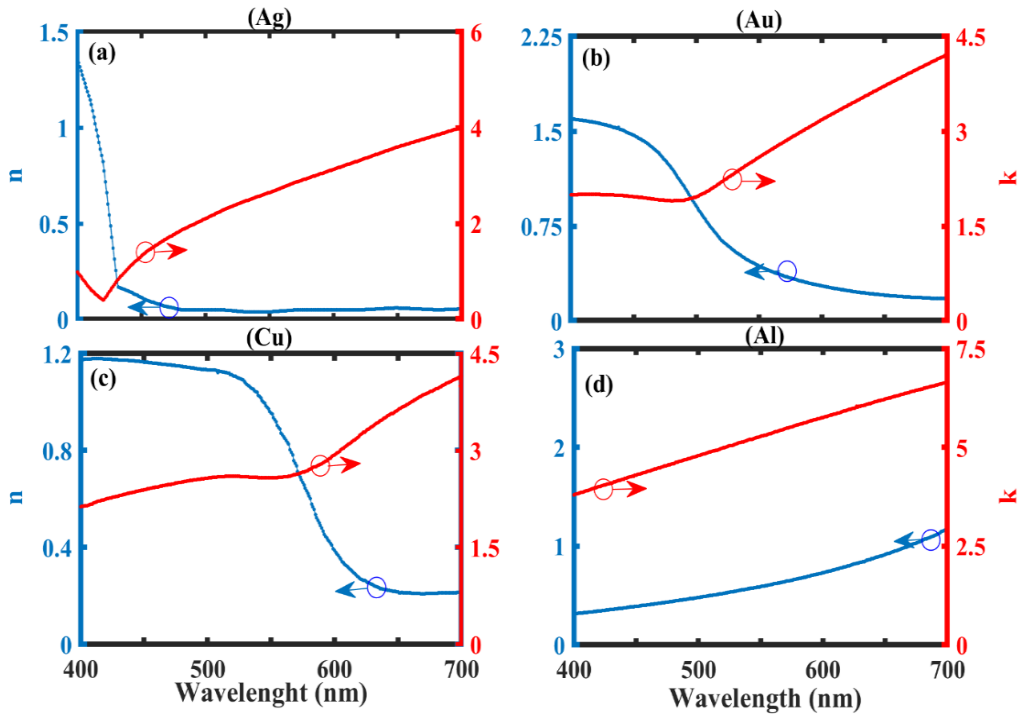


Fig. 3. The n and k refractive index of the (a) Ag, (b) Au, (c) Cu, and (d) Al layer.

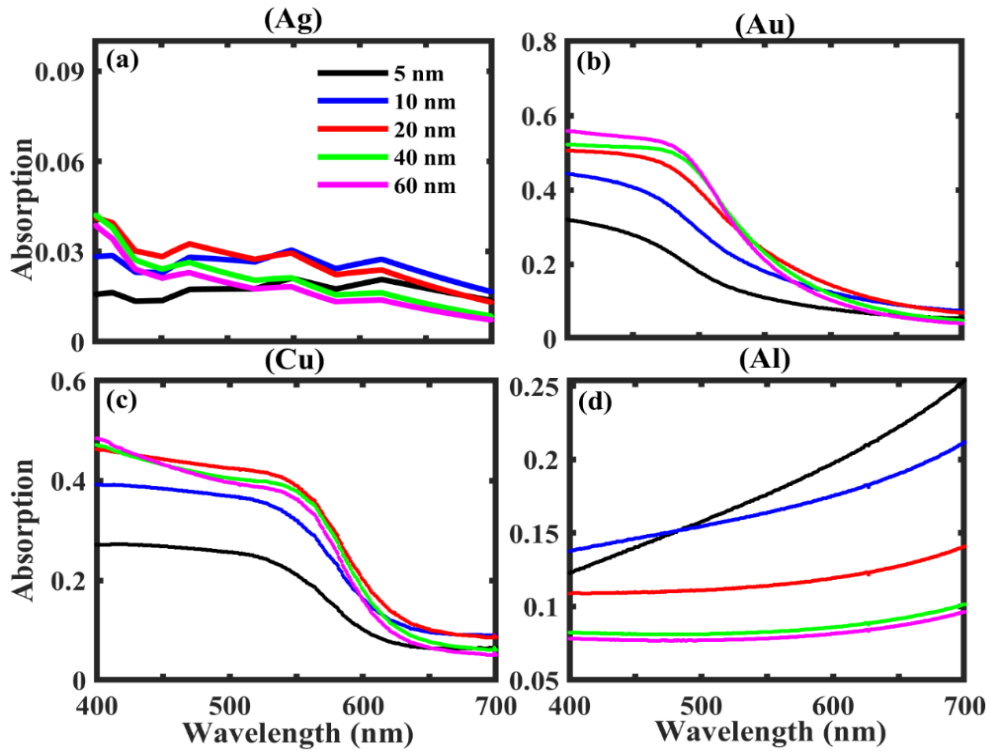


Fig. 4. Absorption spectra for various (a) Ag, (b) Au, (c) Cu, and (d) Al thicknesses.

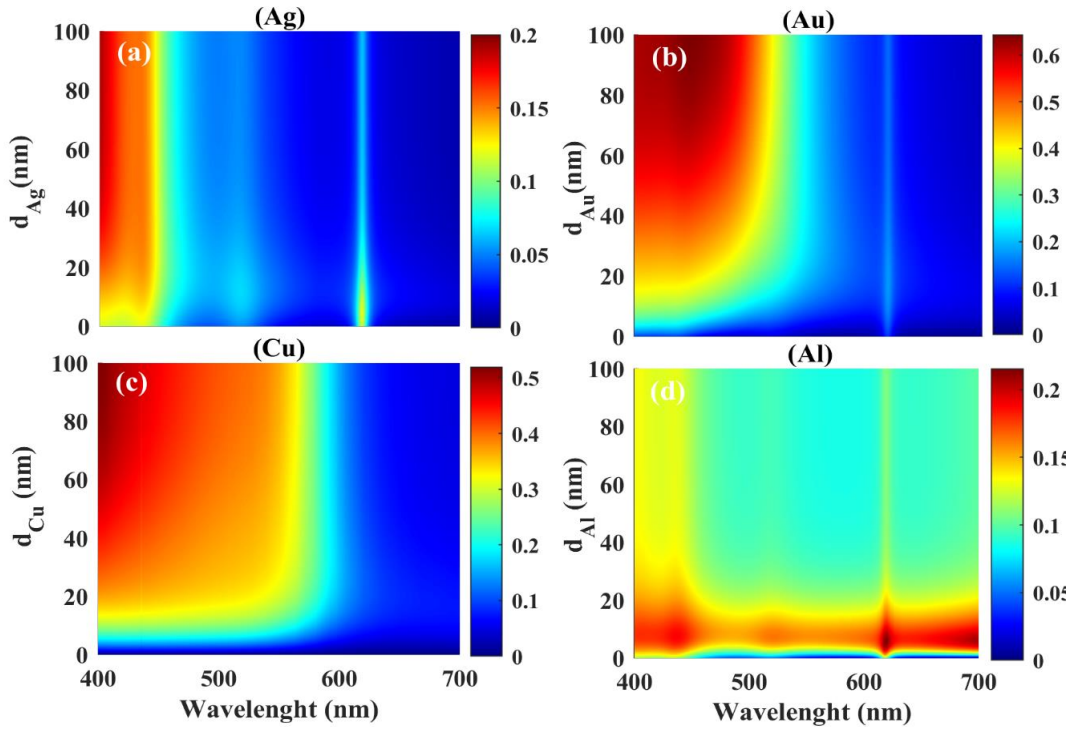


Fig. 5. Absorption as a function of the wavelength and the thickness of the (a) Ag, (b) Au, (c) Cu, and (d) Al layer.

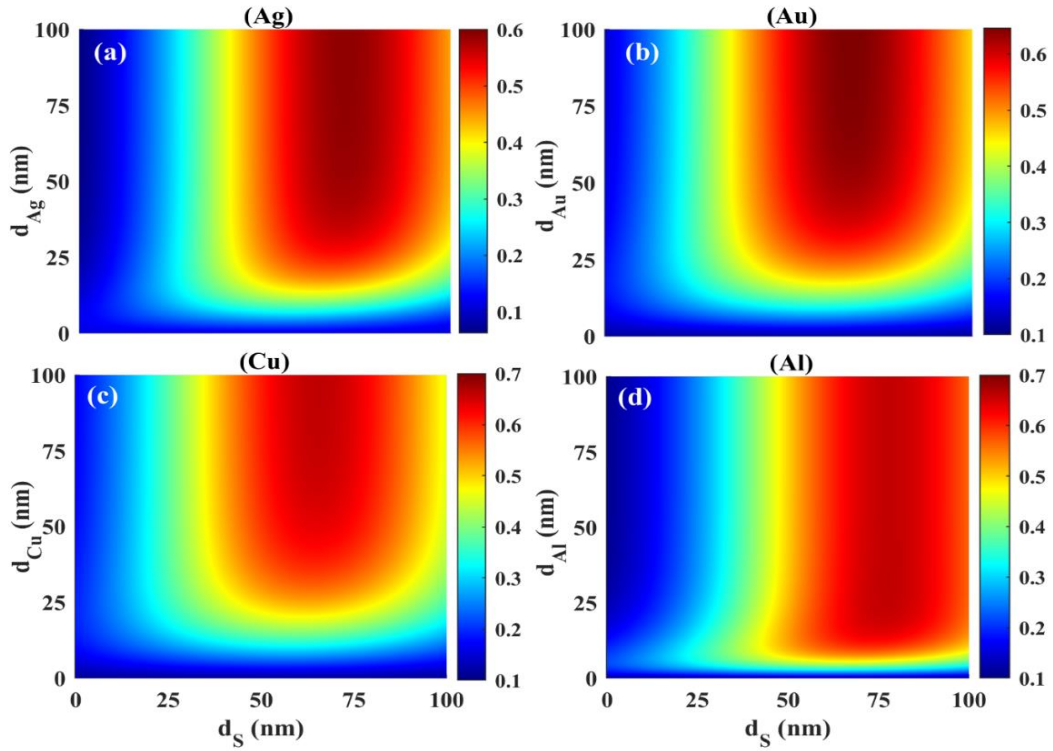


Fig. 6. The absorption as a function of the thickness of the spacer and (a) Ag, (b) Au, (c) Cu, and (d) Al layer at $\lambda=619$ nm.

of absorption which is 18% belongs to $d_{Au} = 16\text{nm}$. Moreover, the absorption decreases slightly with increasing the metal thickness from $d_{Au} = 16\text{nm}$. The absorption of the structure reaches its maximums at 432 and 619 nm which were selected as design wavelengths.

To increase the absorption, we inserted a spacer between the metal layer and WS₂ monolayer. As shown in Fig. 6, the absorption was plotted as a function of the thickness of the spacer and metal layers to determine the optimum thicknesses of achieving maximum absorption at $\lambda = 619\text{ nm}$. The thicknesses of the spacer and metal layers as well as the amount of absorption in optimal cases are given in Table 1. According to Fig. 6d and Table 1 for Al, maximum absorption occurs when $d_s = 75\text{ nm}$ and $d_{Al} = 25\text{ nm}$. An error of about 10 nm is common in the deposition of nanometer layers; this thickness error in the structure under study causes 10% change in the absorption. For example, with an error of 10 nm (5 nm) at a thickness of d_s

$= 75\text{ nm}$, the changes in the amount of absorption would be less than 5% (3%). On the other hand, when the metal thickness error is about 10 nm around $d_{Al} = 20$ ($d_{Al} = 25$), by keeping the thickness of the spacer constant at 75 nm, the absorption value shows almost 10% (5%) variation. Likewise, in Au metal, $d_s = 70\text{ nm}$ and $d_{Au} = 45\text{ nm}$, in Ag metal, $d_s = 70\text{ nm}$ and $d_{Ag} = 40\text{ nm}$, and in Cu metal, $d_s = 65\text{ nm}$ and $d_{Cu} = 50\text{ nm}$ are chosen show less than 5% variation in their absorption.

Similar to Fig. 6, Figure 7 exhibits absorption spectrum as a function of the thickness of the spacer and metal layers at $\lambda = 432\text{ nm}$. The thicknesses of spacer as well as metal layers and the amount of absorption in optimal cases are given in Table 2. According to Fig. 7 and Table 2, by considering the error of the experimental works in making the thickness around 10 nm, $d_s = 45\text{ nm}$ and $d_{Au} = 50\text{ nm}$ are selected in Au metal, $d_s = 40\text{ nm}$ and $d_{Ag} = 60\text{ nm}$ in Ag metal, $d_s = 45\text{ nm}$ and $d_{Cu} = 50\text{ nm}$ in Cu metal, and $d_s = 45\text{ nm}$ and $d_{Al} = 40$

Table 1. The thicknesses of spacer and metal layers and the amount of absorption at $\lambda = 619\text{ nm}$.

Ag			Au			Cu			Al		
d_s	d_{Metal}	A%	d_s	d_{Metal}	A%	d_s	d_{Metal}	A%	d_s	d_{Metal}	A%
60	30	52.57	60	30	55.94	55	35	57.64	65	10	58.26
	35	53.82		35	58.34		40	59.43		15	61.96
	40	54.59		40	59.98		45	60.69		20	62.71
	45	55.07		45	61.11		50	61.57		25	62.69
	50	55.37		50	61.88		55	62.19		30	62.52
	55	55.56		55	62.41		60	62.62		35	62.36
65	30	54.04	65	30	56.32	60	35	58.84	70	10	58.98
	35	55.51		35	58.88		40	60.8		15	63.39
	40	65.43		40	60.66		45	62.18		20	64.56
	45	57.01		45	61.88		50	63.15		25	64.78
	50	57.38		50	62.73		55	63.84		30	64.73
	55	57.61		55	63.31		60	64.32		35	64.64
70	30	54.48	70	30	55.84	65	35	59.14	75	10	58.92
	35	56.13		35	58.49		40	61.20		15	63.88
	40	57.18		40	60.33		45	62.66		20	65.41
	45	57.84		45	61.62		50	63.70		25	65.82
	50	58.27		50	62.5		55	64.43		30	65.88
	55	58.54		55	63.11		60	64.95		35	65.84
75	30	53.91	75	30	54.54	70	35	58.54	80	10	58.11
	35	55.69		35	57.20		40	60.64		15	63.42
	40	56.82		40	59.06		45	62.14		20	65.21
	45	57.55		45	60.36		50	63.21		25	65.77
	50	58.02		50	61.26		55	63.96		30	65.91
	55	58.31		55	61.87		60	64.49		35	65.92
80	30	52.4	80	30	52.53	75	35	57.11	85	10	56.61
	35	54.24		35	55.13		40	59.19		15	64.08
	40	55.43		40	56.95		45	60.68		20	64.02
	45	56.19		45	58.22		50	61.74		25	64.68
	50	56.68		50	59.10		55	62.49		30	64.88
	55	57		55	59.71		60	63.01		35	64.91

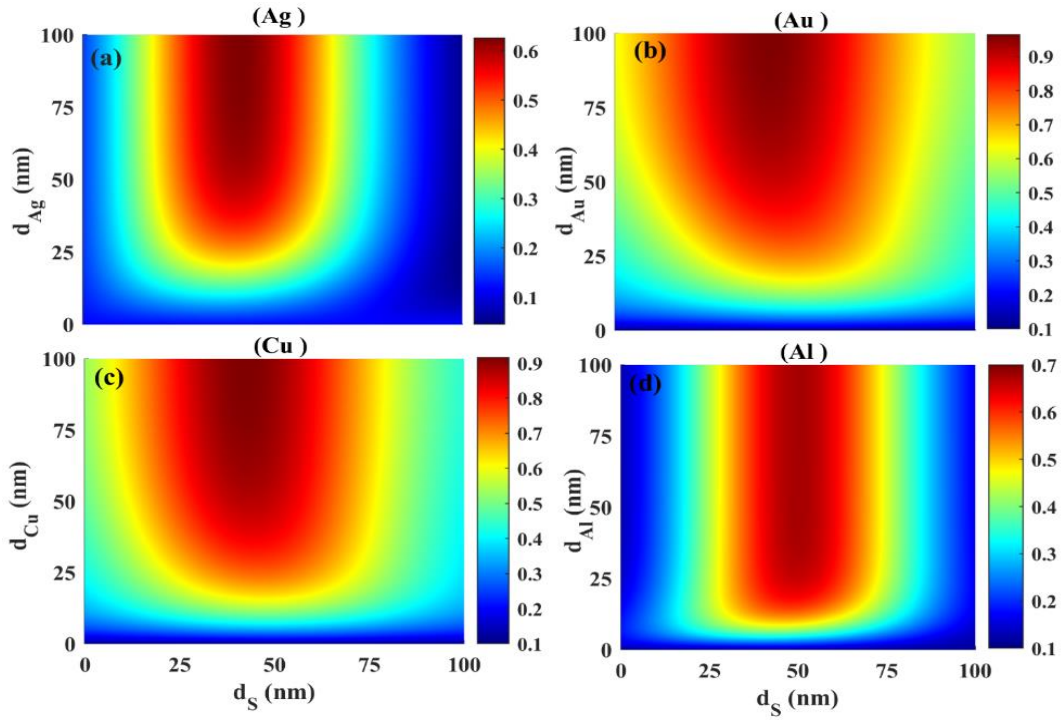


Fig. 7. The absorption as a function of the thickness of the spacer and (a) Ag, (b) Au, (c) Cu, and (d) Al layer at $\lambda=432$ nm.

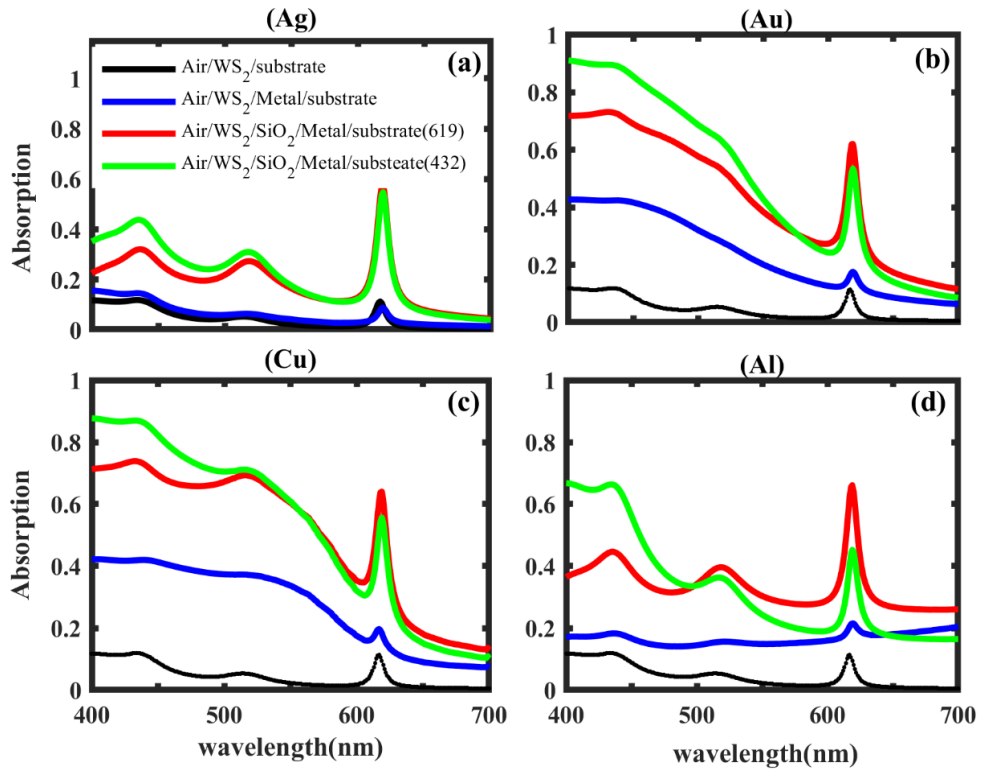


Fig. 8. Absorption spectra for structures air/WS₂/substrate, air/WS₂/ metal/substrate, and air/WS₂/spacer/ metal / substrate for optimal thickness obtained from Table 1 and 2 for (a) Ag, (b) Au, (c) Cu, and (d) Al layer.

Table 2. The thicknesses of spacer and metal layers and the amount of absorption at λ =432 nm.

Ag			Au			Cu			Al		
<i>d_S</i>	<i>d_{Metal}</i>	A%	<i>d_S</i>	<i>d_{Metal}</i>	A%	<i>d_S</i>	<i>d_{Metal}</i>	A%	<i>d_S</i>	<i>d_{Metal}</i>	A%
30	45	52.99	35	30	74.58	35	30	74.66	35	25	56.72
	50	54.03		35	78.78		35	78.04		30	57.06
	55	54.76		40	82.05		40	80.71		35	57.19
	60	55.27		45	84.77		45	82.82		40	57.24
	65	55.63		50	87.01		50	84.48		45	57.26
	70	55.88		55	88.82		55	85.77		50	57.26
	75	56.06		60	90.27		60	86.78		55	57.27
35	45	56.61	40	30	77.21	40	30	76.91	40	25	61.65
	50	57.82		35	81.10		35	80.3		30	62.27
	55	58.68		40	84.28		40	82.93		35	62.55
	60	59.28		45	86.88		45	84.98		40	62.68
	65	59.7		50	89		50	86.57		45	62.74
	70	60		55	90.71		55	87.80		50	62.77
	75	60.21		60	92.06		60	88.75		55	62.79
40	45	58.13	45	30	78.45	45	30	77.78	45	25	64.72
	50	59.45		35	82.18		35	81.06		30	65.58
	55	60.39		40	85.18		40	83.56		35	66
	60	61.05		45	87.61		45	85.48		40	66.2
	65	61.52		50	89.57		50	86.96		45	66.3
	70	61.84		55	91.14		55	88.09		50	66.35
	75	62.07		60	92.40		60	88.97		55	66.38
45	45	57.44	50	30	78.47	50	30	77.22	50	25	65.62
	50	58.80		35	81.94		35	80.28		30	66.66
	55	59.77		40	84.70		40	82.58		35	67.18
	60	60.45		45	86.91		45	84.32		40	67.43
	65	60.93		50	88.69		50	85.65		45	67.56
	70	61.26		55	90.12		55	86.67		50	67.62
	75	61.49		60	91.27		60	87.46		55	67.65
50	45	54.71	55	30	77.29	55	30	75.31	55	25	64.32
	50	56.03		35	80.44		35	78.07		30	65.45
	55	56.97		40	82.90		40	80.11		35	66.01
	60	57.63		45	84.87		45	81.65		40	66.29
	65	58.10		50	86.46		50	82.82		45	66.42
	70	58.43		55	87.75		55	83.72		50	66.49
	75	58.65		60	88.81		60	84.84		55	66.53

nm in Al metal which show less than 5% variation in their absorption.

To determine the optimum structure, absorption spectra of the structures air/WS₂/substrate, air/WS₂/metal/substrate, and air/WS₂/spacer/metal/substrate in the optimal thickness extracted from Table 1 and 2 were plotted in Fig 8. Absorption increased slightly when the metal layer was placed between WS₂ monolayer and the substrate (blue curves) but the maximum absorption was observed when the spacer was inserted between metal and WS₂ monolayer (red and green curves). The absorption of all of four metals was almost equal at λ=619 nm. The amount of absorption of Au and Cu is higher

than that of other metals throughout the visible wavelength range, and thus, these two metals are the best choices for increasing the absorption in this structure.

CONCLUSION

We investigated the effects of different metal and spacer layers to achieve high absorption in a structure consisting of WS₂ monolayer. According to the findings of this study, the maximum absorption was observed when the spacer was inserted between metal and WS₂ monolayer. The absorption increases by employing the optimal thicknesses of metal and spacer layer. Further, the absorption of all of four metals increases

almost equally at $\lambda=619$ nm and the amount of absorption of Au and Cu is higher than of other metals in the entire visible wavelength range. In sum, the results show that our designed structures demonstrate high amounts of absorption which is desirable for optoelectronic applications.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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