



Multi-layer MoS₂-Based Plasmonic Gold Nanowires at Near-Perfect Absorption for Energy Harvesting

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Received: 9 September 2020 / Accepted: 11 February 2021
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Abstract

One of the biggest challenges in relation to the modernistic vision of smart city technology is to provide confident autonomous energy, notably in terms of power storage. If you want to change an existing lifestyle, you cannot ignore the basic concepts collected from basic physics. The subject of Metamaterials stands for an important research area that can be explored and used to come up with unparalleled ideas about the properties and functions that are completely absent from natural materials. In contrast to other bold technologies, combining a simple layered surface with appropriate material selection makes it possible to pattern and manufacture new types of solar cells that work in a wide frequency range. In this article, we propose a simple method to boost the coupling interaction between metallic gold nanowires with multiple MoS₂ layers. The innovation of this work is that the thickness layer changes have great stability in the influence of the absorption performance and electric field distribution in the visible light and near-infrared spectra. Therefore, this new design can be seen as very important in many fields from sensing to solar cell applications.

Keywords Localized surface plasmon resonance · Gold nanowires · 2D materials · Transition metal dichalcogenides

Introduction

Surface plasmons (SPs), induced from collective oscillations of free electrons in the conduction band of metals, are some kind of vanishing waves that are delicate to changes in optical properties in the surrounding medium. It is notorious for the fact that p-polarization will cause charges to be generated at the metal interface and excite SP. This phenomenon occurs when the necessary momentum of incident light is provided through a prism [1] and is commonly referred to as surface plasmon resonance (SPR). Under these specific conditions, the maximum energy of TM

polarized light is transferred to the electrons and produces a sharp peak in the absorption spectrum. This evidence provides the concept of a plasma absorber designed based on metal nanostructures. Nowadays, the system is assigned as a basis for integration into next-generation solar cells to aim smart energy-collecting devices.

Localized surface plasmon resonance (LSPR) is a type of SP related to metal particles whose size is much smaller than the radiation wavelength. The aforementioned basic physics of LSPR has opened up a new way to design metal nanostructures, which has aroused great interest in potential current and future applications. From then on, plasma absorbers have been developed rapidly, and various applications have been found, including biosensors [2–9], dedicated to proteins [10] and the label-free detection of antibodies [11, 12], photoelectric devices [13, 14], to improve the efficiency of photovoltaic cells [15]. In addition, the study of many physical parameters of nanostructures makes it a hopeful promising evaluation for the next generation of fascinating surfaces. Numerical models can be used to optimize and evaluate parameters such as the chemical composition of the substrate on which the metal is deposited, the size and form of the particles, and the surrounding environment to predict its effects. In addition,

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these models allow the development of new materials such as graphene and 2D transition dichalcogenide (TMDs) as molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2) [10, 16, 17].

The interaction between nanoparticles and 2D materials (such as MoS_2) provides further outlooks for optoelectronic applications. In the sub-nanometer distance, due to the tunneling effect of electrons between the metal nanoparticles and the active semiconductor layer, other functions also play a role. MoS_2 is a two-dimensional nanomaterial containing a hexagonal crystal lattice, in which atoms bind together by a strong linking of force and layer composite by van der Waals forces. From a plasmon perspective, compared with other materials, MoS_2 has supporting optical and tribological properties. First, concerning electron distribution, MoS_2 has tribological properties including an almost zero friction or super-lubrication state. Secondly, MoS_2 has higher thermal stability and oxidation resistance. Finally yet importantly, nanoscale MoS_2 has a very elevated density, small size, large specific surface area, and a high specific surface energy.

Recently, many studies [18, 19] [20, p. 2] [21, 22] have been conducted to show that the integration of these monoatomic coating above the substrate allows a significant enhancement of the optical properties such as absorption [23], light emission [24], and photoluminescence [25]. However, studies on interactions using multi-layer TMDs have rarely been reported in the literature. Additionally, unlike the systems found in the literature, the simplicity of the design makes it easy to reduce difficulties for experimental realizations and with large absorption factors.

In this work, we report on a numerical study using the finite element method (FEM) and the Drude-Lorentz model to predict accurately the optical signature of a gold nanowire anchored onto MoS_2 surfaces. A particular attention is given to the influence of MoS_2 on the performances. By studying several MoS_2 thickness parameters, we highlighted the optimum configuration trade off; maximum absorption versus frequency range of operation.

This paper is structured as follows: in “[Structure and Modeling Method](#),” the structure and the modeling method

used in this study are presented in detail. In “[Results and Discussion](#),” we address the results and discussions around several parameters and the design performances. The conclusion is given in “[Conclusions](#).”

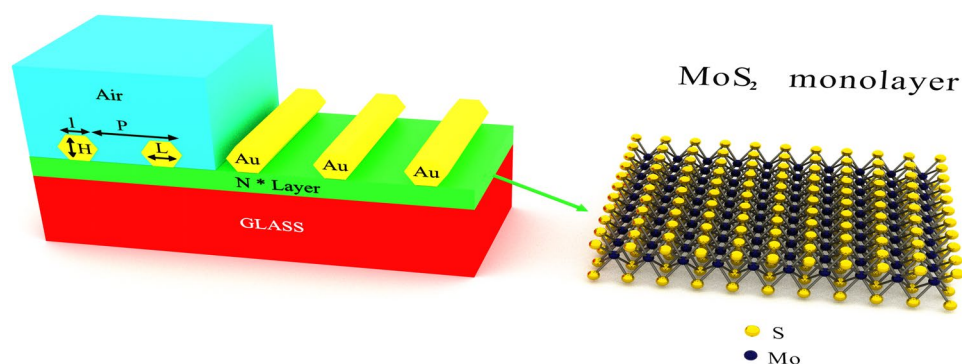
Structure and Modeling Method

The numerical results are implemented by using the finite element method (FEM) with the COMSOL Multiphysics software. Our calculations were undertaken in a 2D model (along the x - and y -axes) by considering the propagation along the y -axis. The two boundaries (where the incident wave is defined and collected) correspond to port boundary conditions. This system of boundary conditions makes it possible to determine the elements of the S-matrix and thus to deduce therefrom the transmission, reflection, and absorption coefficients.

We applied the periodic boundary condition along the x -direction to simulate an infinite unit cell (see Fig. 1), and the structure is set to be with infinite size in the z -direction. The modeling space is discretized using a triangular mesh. The minimum mesh size inside the MoS_2 is equal to 0.1 nm. The input optical field, with a polarization direction of the transverse magnetic (TM) mode, is excited at the top part of the unit cell by a light source along the y -axis. The transmission spectra of the optical signal, detected at the bottom side of the unit cell, are collected in terms of the optical frequency. The absorption of the proposed structure can be given as follows: $A = 1 - R - T$, where R and T are the reflection and transmission spectra of the proposed structure. All the absorption spectra are normalized with respect to the problem.

The plasmonic nanostructures investigated in this work are assembled with Au nanowires in hexagonal shapes. This hexagonal Au nanowire array designed here is configured by the height of H , the two diameter parameters of l and L , and where p is for the period pitch (see Fig. 1). This hexagonal nanowire periodic structure is arranged upon a N layer of

Fig. 1 3D sketch of MoS_2 -based nanostructure



MoS₂ ($d_{\text{MoS}_2} = N \cdot d = N \cdot 0.646 \text{ nm}$). The thickness of the monolayer MoS₂ has been previously measured experimentally by Li et al. [26]. The dispersion of MoS₂ was retrieved from the transmission measurements using a multi-Lorentzian model [26]. The absorption bands were represented by multiple resonances as:

$$\epsilon(E) = \epsilon_B + \sum_{j=0}^N \frac{f_j}{E_{0j}^2 - E^2 + iE\Gamma_j},$$

E represents the photon energy in eV, where ϵ_B , f_j , E_{0j} and Γ_j are respectively the non-resonant background dielectric permittivity, oscillator strength, resonance center energy, and the phenomenological damping constant of the absorption band j . All these parameters were varied to fit to experimental measurements. All details regarding the fitting process applied to the visible spectra were extracted from reference [27]. The parameter values are given in Table 1.

Finally, the MoS₂ was formed on a glass surface whose refractive index is estimated at 1.5 (Fig. 1). In the first part of this study, we have employed a light source with a normal incident angle as the excitation fields. After that, we changed the wavelength across the visible range in order to collect the localized SPR spectra of the metallic structures by optimizing both the periodicity and thickness of the TMD material.

The dielectric constant of gold nanoparticle is described by the Lorentz-Drude model. In the complex permittivity frequency-dependent analysis of metals [28], this model will allow us to fit experimental measurement data for the optical frequency-dependent dielectric parameters of metals with real and imaginary parts, in a relatively high precision in the visible range ($350 < \lambda < 900 \text{ nm}$).

Results and Discussion

In order to maintain the shape of the designed hexagonal structure, the parameter L in these configurations should be larger than the value of parameter l . For the sake of simplicity, we have chosen $L = l + 10 \text{ nm}$ in the modeling. These geometrical parameters of the hexagonal

nanowires are defined according to the experimental and numerical data in the literature [29], so the optimized parameters are: $l = 30 \text{ nm}$, $L = 40 \text{ nm}$, and $H = 15 \text{ nm}$. Firstly, we evidenced strong absorption enhancement of MoS₂-based hexagonal gold nanostructure by means of plasmonic gold (Au) nanorods. Figure 1 shows the schematic structure consisted of 2D MoS₂ layers and gold nanowires. Through an appropriate design of gold nanowires displaying an LSPR frequency near the direct band gap of MoS₂ (1.86 eV), the localized SPR generated by the presence of Au nanowires will spectrally and spatially be coupled to the emission of the MoS₂ layers. And this strong coupling effect will result in a large enhancement at the optical absorption. Therefore, the geometrical parameters of gold nanowires have to be optimized to perform substantial absorption.

It is well known in the field of plasmonics that periodicity of the plated gold nanowires would significantly influence the optical signature. Thus, our first concern was about to tune absorption for several periodicities with values ranging from 50 to 90 nm in order to understand the influence of periodicity p on the plasmonic resonance. Figure 2 displays the obtained results in which the best value is noticed to be optimum around $p = 50 \text{ nm}$.

To further study the influence of the structure's geometry, it is also important to investigate the effects on changing the pitch period p . It is worth noting that the localized effect could be observed through the absorption spectrum for the light with TM modes. Effectively, as the particle distance was decreased, the optical resonance of the structure becomes significantly strong in the light interaction; when the period of the particle array (p) was 50 nm, a strong optical absorption of light energy (77%) was shown. The absorption enhancement due to the periodicity is varying from 42% ($p = 90 \text{ nm}$) to 77% ($p = 50 \text{ nm}$). When the distance between the particles becomes smaller, the mutual influence of particles reveals a stronger electric field coupling effect. Thus, this fact results in an electric field enhancement that can be explained by the fact that the excited electric field is generated by the double interactions through the incident field and the resonance between nanowires. This underlying physics explains our choice of the parameter $p = 50 \text{ nm}$. Let us now mention that when p varies from 50 to 90 nm, the resonant wavelength decreases and shifts to step to the blue range. These results are confirmed with experimental works in the literature for the same systems [30]. It should be noted that for a weaker coupling regime between metallic nanostructures with a larger value of particle period p , the change of p value would not have any effects on the plasmonic resonance of the particles. Therefore, within the limits of an experimental realization, the small

Table 1 The MoS₂ dispersion parameter values (see Ref. [27])

Oscillateur j	f_j	$E_j(\text{eV})$	$\Gamma_j(\text{eV})$
1	0.65	1.9001	0.040
2	0.25	1.9315	0.050
3	1.2	2.0516	0.080
4	5	2.3065	0.8
5	12	2.4	1
6	24	2.87	0.35

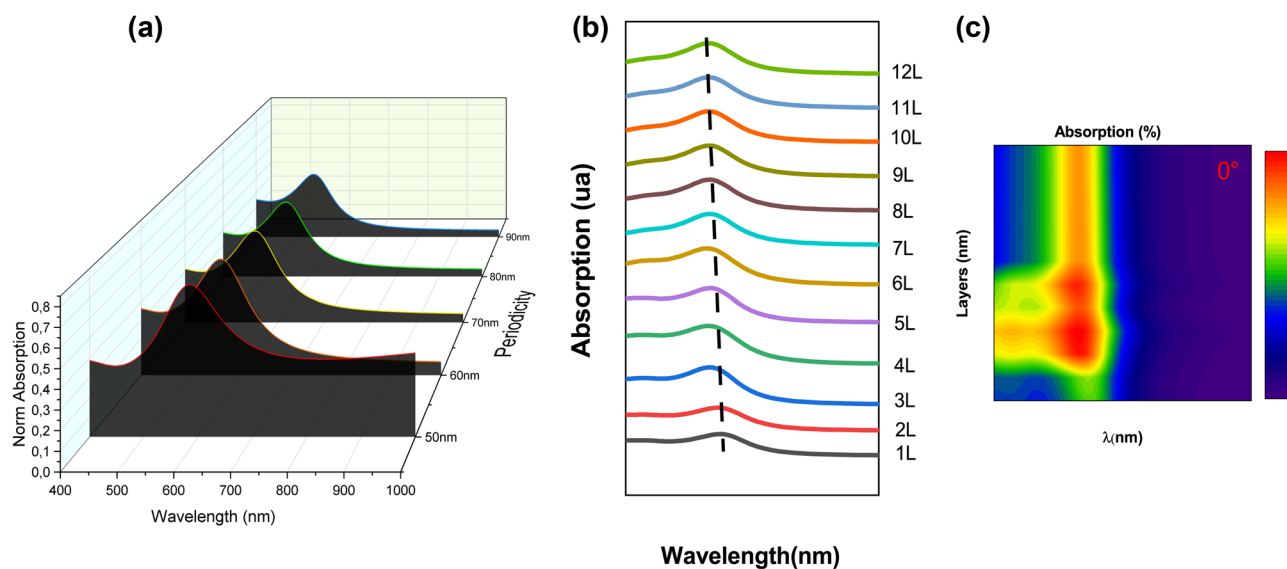


Fig. 2 (a) Evolution of the absorption coefficient of hexagonal gold nanowires along with period p without MoS₂ layers. (b) Absorption spectrum of the studied structure for several MoS₂ layers. (c) Color

map of absorption as function of the wavelength (x -axis) and the layers (y -axis), illuminated by TM polarization for normal incident case

value of p allows this plasmonic structure concentrate and absorbs the light in the sub-wavelength volumes, which are of great interest for plasmonic solar cells. Compared with the gold rectangular ribbon structures, a stronger plasmonic effect can still be observed. This is due to hexagonal geometry that might support a stronger electric field localization at the edges of the Au NPs that are more flexible and easier to be excited in our structure compared with rectangular ribbons.

Based on the results in Fig. 2a, it can be seen that periodicity has an impact on the absorption in which we performed an enhancement from 42 to 77%. Now, we added the potential MoS₂ 2D material as a spacer between glass and nanowires as they are promising materials in plasmonics. We plot the evolution of the absorption spectra with varying number of MoS₂ layers at normal incidence (Fig. 2b). Thus, we can see a blue shift of 31.5 nm between 1 and 12L. As shown in Fig. 2c, the maximum absorption is observed between 3 and 6L. For 3L of MoS₂, the absorption coefficient can reach 94.95% at 537.8 nm to 98.2% at 527.7 nm for 4L. We can notice that the optical absorption of the overall structure for the given wavelength region is significantly improved as function of MoS₂ layers.

After that, we also studied the dependence of the optical absorption for the designed MoS₂-based hexagonal gold nanowires on geometrical parameters p and H . The variation

of the absorption for different layers of MoS₂ as function of the period p is presented on Fig. 3.

Similarly to the previous case (without 2D material: Fig. 2a), the period effect of the gold nanowires to the absorption spectra remains the same. By changing the period p from 50 to 80 nm, the absorption spectrum shifted to a shorter wavelength, and maximal absorption will decrease with increasing of the period, which is due to the fact that the coupling with LSPR arrays will low coupling between nanowires when the period increases. The red color in Fig. 3a manifests the strong absorption in the range from 3 to 6L.

Based on the observation of the above results, the maximal absorption has been remarkably decreased with period p to 98%, 81%, 70%, and 43% at 50 nm, 60 nm, 70 nm, and 80 nm, respectively.

In parallel, we investigate the dependence of the absorption according the thickness H of MoS₂-based hexagonal gold nanowires. As is well known, the LSPRs are very sensitive to changes of geometrical parameters. Figure 4 shows the effect of the thickness H of the nanowires. We noticed also an optical shift toward shorter wavelengths with an increasing H , while a decrease for the maximal absorption was observed which shows a high plasmonic sensitivity for smaller height values, especially for $H = 10$ nm. The optimal absorption value based on numerical simulations (99.6%) is observed for $H = 10$ nm

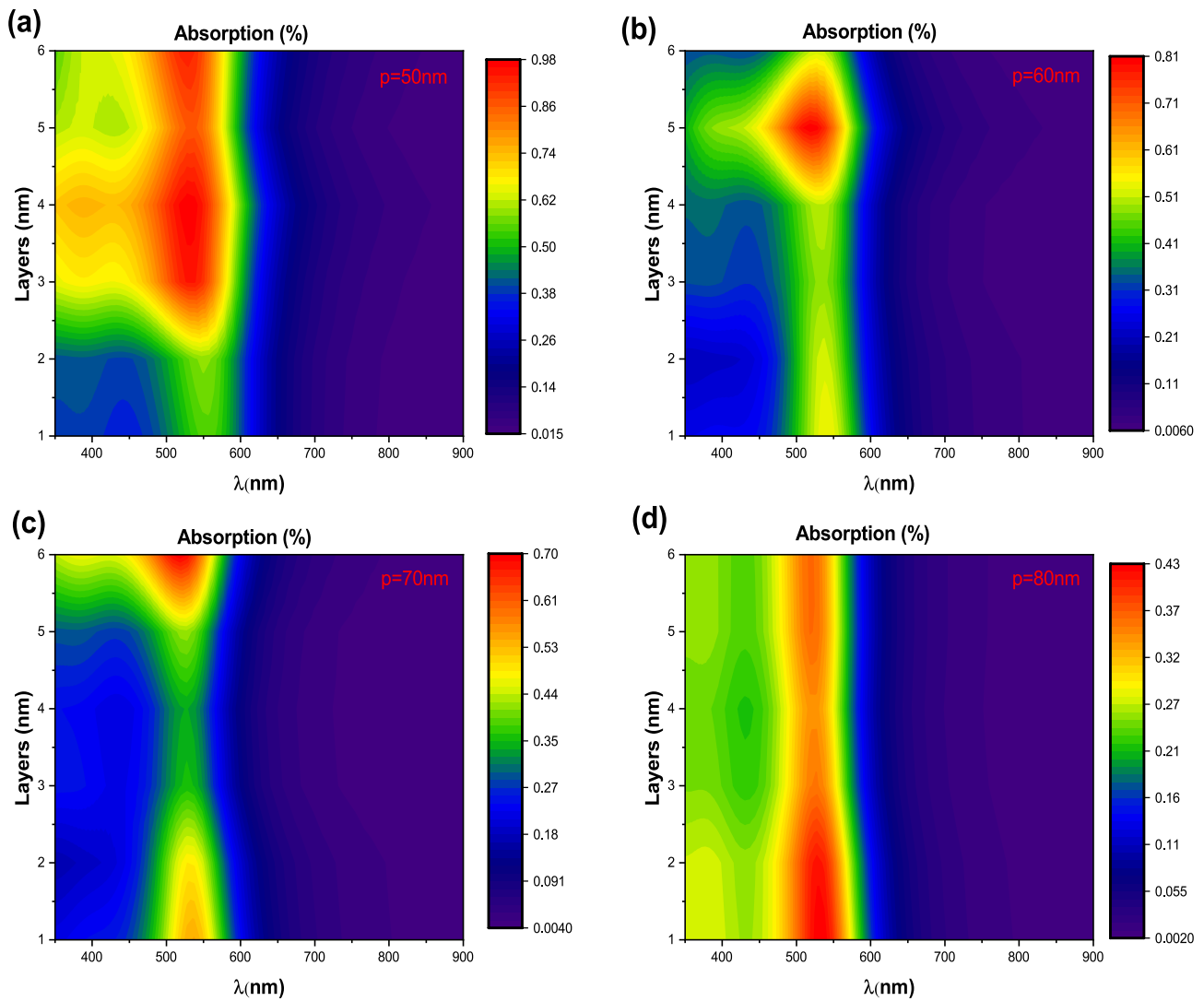


Fig. 3 Color map of absorption for different MoS₂ layers as a function of period p . (a) $p=50$ nm. (b) $p=60$ nm. (c) $p=70$ nm. (d) $p=80$ nm. The remaining geometrical parameters are held constant such as $l=30$ nm, $L=40$ nm, and $H=15$ nm

for 3L of MoS₂ at 559.24 nm (Fig. 4a). Note that the height H does not modify notably the maximal absorption, since a weak decay of 6.6% is observed in the maximal absorption when the particle height value was changed from 10 to 25 nm.

Subsequently, we have investigated the optical absorption of the MoS₂-based hexagonal gold nanowires at oblique incidence, in order to understand the effect during the presence of 2D material on the absorption enhancement. One can see in figure 5 that the maximal absorption of the proposed MoS₂-based hexagonal gold nanowires remains the same with incident angles increasing from 10° to 40° for TM polarization. Additionally, at 40°,

the maximal absorption is increased for all MoS₂ layers. This fact provides both good absorption and optical stability under oblique incidence. The proposed design offers the advantage of being flexible as opposed to the showcased complicated geometries in the literature. The flexibility and simplicity of the designed structure will definitely benefit the future design of energy-harvesting nanophotonic and optoelectronic devices.

In the end, we try to provide an analysis of near-perfect absorption through the impedance transformation approach for optimal parameter value previously treated. This condition is satisfied, when the impedances of the nanowires have almost been equal to 1 (i.e., free space impedance).

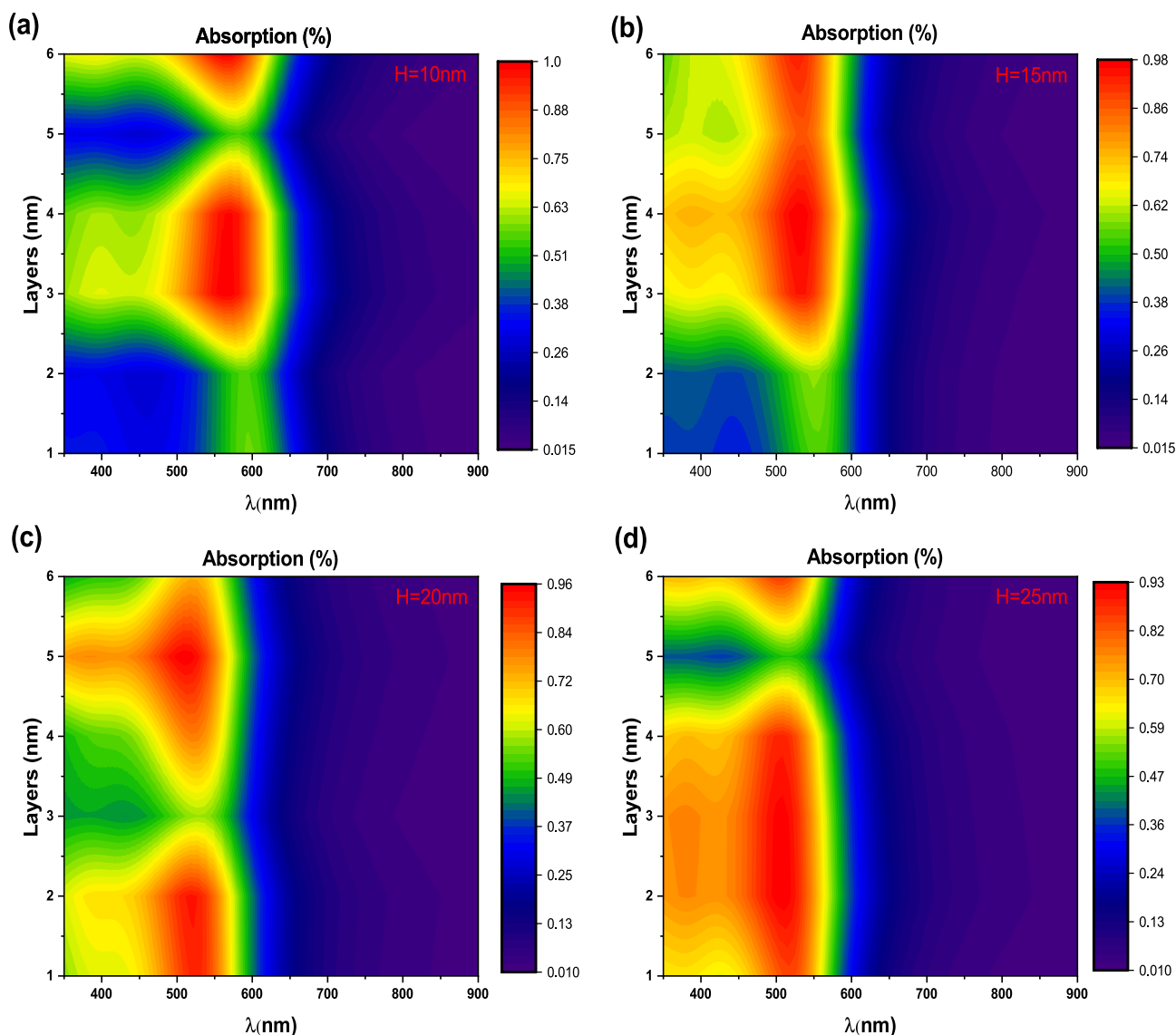


Fig. 4 Color map of absorption for different MoS₂ layers as a function of H. (a) H=10 nm. (b) H=15 nm. (c) H=20 nm. (d) H=25 nm. *l*=30 nm, *L*=40 nm, and *p*=50 nm

The blue line in Fig. 6a shows the localized SPR spectra of 3 layers of MoS₂ with the wavelengths ranging from 350 to 900 nm, and the localized SPR has been significantly improved. In order to calculate the impedance (*Z*), the relation between the S (*S*₁₁ and *S*₂₁) parameters and *Z* can be easily derived with both relations [31, 32]:

$$S_{11} = \frac{i}{2} \left(\frac{1}{Z} - Z \right) \sin(nkH) \tag{1}$$

$$S_{21} = \frac{1}{\cos(nkH) - \frac{i}{2} \left(\frac{1}{Z} + \frac{1}{2} \right) \sin(nkH)} \tag{2}$$

where *n*, *k*, and *H* represent the effective refractive index, the electromagnetic wave vector, and the nanostructure thickness, respectively.

Therefore, the impedance is given by:

$$Z = \pm \sqrt{\frac{(1 + S_{11})^2 - S_{21}^2}{(1 - S_{11})^2 - S_{21}^2}} \tag{3}$$

The condition to be satisfied to achieve a near-perfect absorption is that the impedance at the resonance wavelength at working range should be near to the free-space impedance (*Z*=*Z*₀) [31, 32].

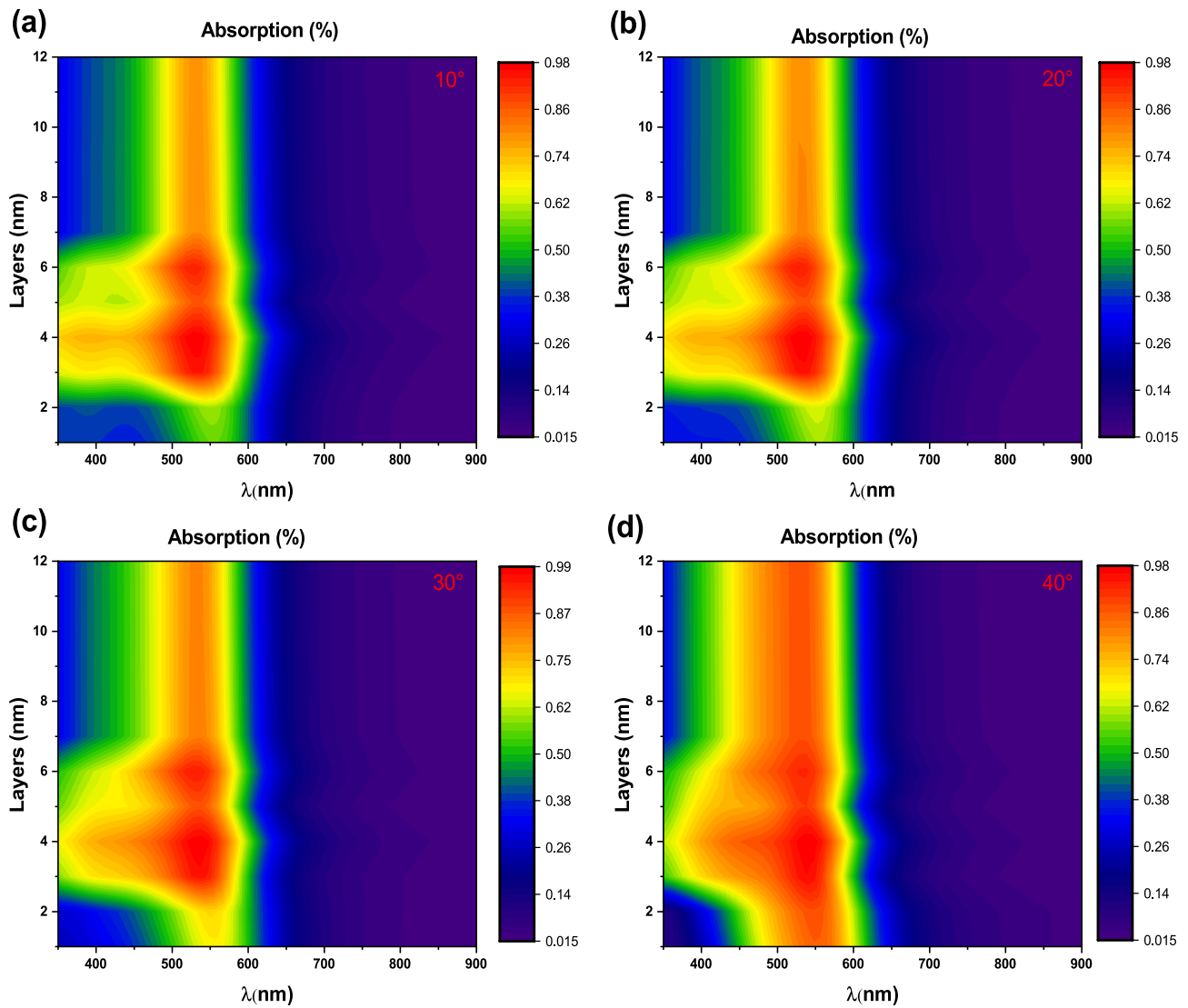


Fig. 5 Color map of absorption for different MoS₂ layers as a function of incident angle. (a) 10°. (b) 20°. (c) 30°. (d) 40°. $l=30$ nm, $L=40$ nm, and $p=50$ nm

We notice at Fig. 6b that the impedance of the designed MoS₂-based hexagonal nanowires is close to 1 at the resonance wavelength of $\lambda_R = 559.24$ nm, which perfectly agreed with the near-perfect absorption.

This observation is confirmed by the field maps presented in Fig. 6c, where we show the electric and magnetic field amplitude distributions at the resonance ($\lambda_R = 559.24$ nm). Therefore, we can see that around the interface between hexagonal nanowires and MoS₂, the electric field and magnetic field are harvested and enhanced.

The hot spots in each of nanowire corner, and especially the two corners directly attached with TMD active layers, generally induce the losses due to the localized field intensity. In our design, the interface between gold hexagonal nanowires and the MoS₂ multilayers allows to trap and absorb light in high efficiency. This strong absorption is due to high concentration of the light energy and near-field enhancement in MoS₂ multilayers by the strong confinement through the LSPR mode located in the interface of gold nanoparticles and their corner edges.

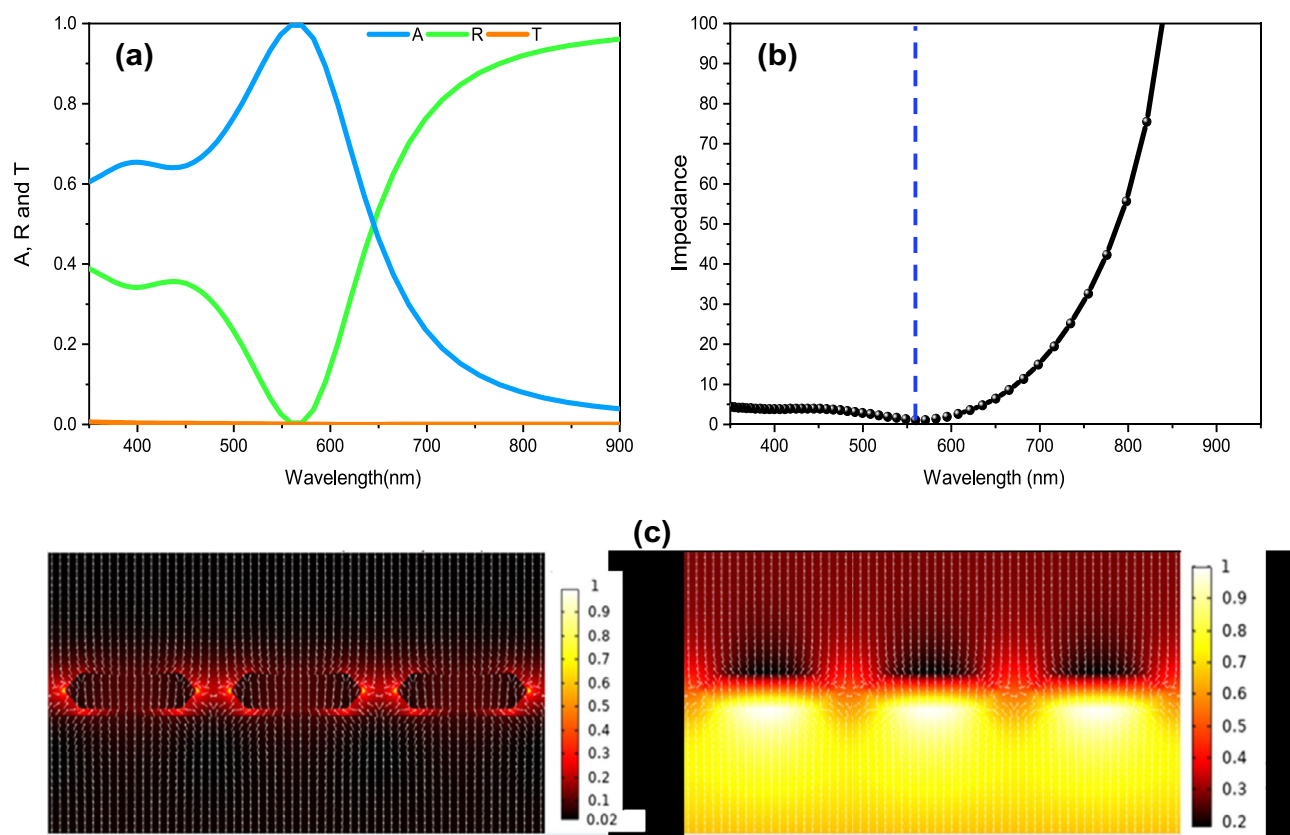


Fig. 6 (a) Absorption (A), reflection (R), and transmission (T) for optimal parameter (3L of MoS₂, $H=10$ nm, $p=50$ nm, $L=40$ nm, and $l=30$ nm). (b) Impedance of the MoS₂-based hexagonal nanowires.

(c) The electric field $|E|$ and magnetic field $|H|$ amplitude distribution at resonant wavelength $\lambda_R = 559.24$ nm. The white arrow is corresponding to the Poynting vector

Conclusions

In this work, a theoretical study is done to observe the effect of MoS₂ TMDs material, on the absorption coefficient and electric field distribution of a new 2D hybrid plasmonic nanostructure. The designed nanostructure is structured by a gold nanowire with hexagonal shape deposited on N layer of MoS₂ TMD material. It is demonstrated that the combined influence of MoS₂ multi-layers and gold nanowire array has significantly increased the light transmitted by the 3 layers of MoS₂, and a strong localized field concentration was achieved to enhance the optical absorption. From our results, we found that in the presence of MoS₂, the absorption of the nanostructure can reach above 99.6%. The proposed nanostructures based on the hexagonal gold nanowire with MoS₂ TMDs active layers would be a best choice for the optical nanodevices.

Acknowledgements A. Akjouj gratefully acknowledges the hospitality of the department of Physics, Faculty of Science, University of Moulay Ismail of Meknes. This work was partially supported by the program FINCOME “Centre National pour la Recherche Scientifique et Technique, Morocco”.

Author contribution All calculations and writing: Z.O. Supervision of the work: A.A., A.M. Substantial contributions to the scientific discussions: S.Z, Y.A. All the authors have read and accepted the version of the manuscript.

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