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RESEARCH ARTICLE

Kretschmann configuration as a method to enhance optical absorption in two-dimensional graphene-like semiconductors

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Abstract
Objectives. The optical properties of two-dimensional semiconductor materials, specifically monolayered transition metal dichalcogenides, present new horizons in the field of nano- and optoelectronics. However, their practical application is hindered by the issue of low light absorption. When working with such thin structures, it is essential to consider numerous complex factors, such as resonance and plasmonic effects which can influence absorption efficiency. The aim of this study is the optimization of light absorption in a two-dimensional semiconductor in the Kretschmann configuration for future use in optoelectronic devices, considering the aforementioned phenomena.
Methods. A numerical modeling method was applied using the finite element method for solving Maxwell's equations. A parametric analysis was conducted focusing on three parameters: angle of light incidence, metallic layer thickness, and semiconductor layer thickness.
Results. Parameters were identified at which the maximum area of absorption peak was observed, including the metallic layer thickness and angle of light incidence. Based on the resulting graphs, optimal parameters were determined, in order to achieve the highest absorption percentages in the two-dimensional semiconductor film.
Conclusions. Based on numerical studies, it can be asserted that the optimal parameters for maximum absorption in the monolayer film are: Ag thickness <20 nm and angle of light incidence between 55° and 85°. The maximum absorption in the two-dimensional film was found only to account for a portion of the total absorption of the entire structure. Thus, a customized approach to parameter selection is necessary, in order to achieve maximum efficiency in certain optoelectronic applications.

Keywords: two-dimensional semiconductors, transition metal dichalcogenides, surface plasmon resonance, plasmon effects, nanostructured metal films

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НАУЧНАЯ СТАТЬЯ

Конфигурация Кречмана как метод увеличения оптического поглощения в двумерных графеноподобных полупроводниках

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Резюме
Цели. Оптические свойства двумерных полупроводниковых материалов, в частности монослойных дихалькогенидов переходных металлов, предоставляют новые возможности в области нано- и оптоэлектроники. Однако практическое применение этих материалов ограничено из-за низкой способности поглощать свет, вызванной их высокой прозрачностью. При работе с такими тонкими структурами возникает возможность использования множества физических механизмов, включая резонансные и плазмонные эффекты, которые можно настроить для улучшения эффективности поглощения света. Цель данной работы – оптимизация поглощения света в двумерном полупроводнике в конфигурации Кречмана с учетом указанных выше явлений для последующего применения в устройствах оптоэлектроники.
Методы. Для проведения моделирования использован метод конечных элементов решения уравнений Максвелла в структуре, представляющей стандартную конфигурацию Кречмана. Проведен параметрический анализ влияния трех параметров: угла падения света, толщины металлического слоя и толщины полупроводникового слоя.
Результаты. Проведено исследование конфигурации модели Кречмана с целью достижения максимального оптического поглощения в двумерной полупроводниковой пленке. Определены параметры, при которых наблюдается наибольшая «площадь» пика поглощения, включая толщину металлического слоя и угол падения излучения. На основе полученных результатов выявлены лучшие параметры для достижения наивысшей степени поглощения в двумерной пленке полупроводника.
Выводы. На основе численных исследований конфигурации модели Кречмана обнаружено, что оптимальными параметрами для максимального поглощения в монослойной пленке являются: толщина слоя серебра, не превышающая 20 нм, и угол падения света от 55° до 85°. Установлено, что максимальное поглощение в двумерной пленке составляет лишь часть от общего поглощения всей структуры. Таким образом, для достижения максимальной эффективности в определенных оптоэлектронных приложениях необходим индивидуальный подход к выбору параметров.

Ключевые слова: двумерные полупроводники, дихалькогениды переходных металлов, поверхностный плазмонный резонанс, плазмонные эффекты, наноструктурированные металлические пленки

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INTRODUCTION

Despite the unique properties of two-dimensional semiconductor materials, their integration into nano- and optoelectronics devices still remains a significant challenge. For example, monolayer transition metal dichalcogenides (TMD) such as MoS_2, $MoSe_2$, WS_2, WSe_2, and others, although being promising for application in optical detectors and photovoltaic elements, have a significant disadvantage that stems from their two-dimensionality, i.e., high optical transparency. In [1], it was demonstrated that the two-dimensional MoS_2 film absorbs no more than 10% of the incident light in the visible optical range. This is not sufficient for creating effective photosensitive elements on their basis. However, the most obvious solution to this problem, which consists in increasing the intrinsic thickness of the semiconductor, cannot be realized due to the almost instantaneous transition from direct-bandgap to indirect-bandgap semiconductor. This can lead to the subsequent loss of its efficiency as a photosensitive element.

At present, this problem can be solved using various approaches. These approaches can be conventionally divided into two main groups. The first group uses interference effects arising from the Fabry–Perot resonator [2–4], while the second group relies on the use of local or surface plasmon resonances [5–10].

Thus, the paper [3] shows that light absorption in a two-dimensional MoS_2 film can reach 70%, and in the WSe_2 75%. This is due to the inclusion of a layer of hexagonal boron nitride in the resonator. Paper [11] demonstrates a twofold theoretical and sixfold experimental increase in the absorption of a two-dimensional MoS_2 film in almost the entire visible spectrum when the structure is changed from $MoS_2/SiO_2/Si$ to $MoS_2/SiO_2/Au/Si$. This is due to the occurrence of interference due to multiple reflections from the air/SiO_2 и SiO_2/Au interfaces.

Despite the need for much more sophisticated technological methods and approaches to utilize plasmonic effects, they are often more effective. For example, in the use of nanoparticles or plasmonic antennas, there is a resonant amplification of the electromagnetic field at the metal/semiconductor interface, making it possible to concentrate light directly into two-dimensional structures [5]. Repeated attempts have been made over the past few years to enhance the photoluminescence signal in monolayers of TMD (e.g., such as MoS_2, WS_2, and WSe_2) by depositing single metallic nanoparticles or arrays of them on the surface of the TMD [6, 7]. Due to its relative simplicity compared to other technological methods for creating plasmonic structures, this method can be used to develop photosensitive devices [12, 13].

Many experimental and theoretical works are devoted to ordered plasmonic structures deposited on two-dimensional semiconductors [8–10]. One of their key advantages is the possibility of adjusting the performance characteristics of optical devices by modifying the shape and geometry of plasmonic elements [14, 15].

The possibility of combining plasmonic and interference techniques is also worth noting. This is confirmed by the results published in [16]. An absorption of 40% in the MoS_2 monolayer in the visible range was obtained using a combination of interference dielectric coating and nanoscale grooves. Also, [17] showed a method for creating ordered silver plasmonic structures on the surface of a waveguide. Nearly 95% total absorption in the entire structure (and 70% absorption in the MoS_2, monolayer in particular) was demonstrated by using a geometry that combines interference and plasmonic effects.

All the above-mentioned methods are based on the effect of local plasmon resonance, involving absorption in metallic plasmonic nanostructures, which is not optimal. Under certain conditions, surface plasmon resonance can be devoid of these drawbacks. To date, several papers have been presented which show the advantages of using surface plasmon resonance in Kretschmann geometry [18, 19]. In [20], high absorption in TMD (reaching almost 100%) was obtained by depositing a two-dimensional TMD film directly onto the dielectric surface. A standing plasmon wave propagates along the semiconductor/dielectric interface, due to which the incident radiation is localized in the TMD and its total absorption increases. It should be noted that in this work, high absorption is achieved not in the two-dimensional TMD film itself, but in the entire structure, including a periodic strip plasmonic lattice of gold.

However, to date, the use of Kretschmann geometry to enhance optical absorption in TMD has not yet been developed to an applied level. Since it is fundamentally technologically simpler than the creation of plasmonic structures by lithographic methods, its successful application requires more theoretical studies to optimize its use in combination with two-dimensional semiconductor films. In this case, the very physical mechanism of optical radiation detection in the structures described above is important. In these structures, the greatest contribution to the photocurrent is made by the photovoltaic effect and photoconductivity effect [21–23] which occur in the nanoscale layer of TMD itself. Thus, for the photosensitive elements created, the main role is played not by the total absorption in the created multilayer structures, but by the absorption in the TMD itself, which, obviously, can already be much lower. This work is devoted to the theoretical modeling of the application of Kretschmann geometry, in order to estimate the possibility of increasing the absorption in a two-dimensional semiconductor layer rather than in the whole structure, which is especially relevant for photovoltaic applications.

METHODS AND APPROACHES

A simulated structure consisting of a glass prism with refractive index approximately equal to 1.5 [24, 25], onto which a thin metal layer and a two-dimensional TMD film were deposited (Fig. 1). Metals such as gold [26, 27], copper [28, 29], aluminum [30], or platinum [31] are commonly used in the Kretschmann configuration. In order to generate plasmon waves of the highest intensity, a material must be chosen with the largest modulo value of ε´ (real part of the dielectric constant) and small value of ε´´ (imaginary part of the dielectric constant) in the chosen visible optical range [30]. In this case, silver is the optimal choice. It should be noted that copper and gold show slightly lower efficiency in the selected wavelength range. However, the use of gold is not commercially feasible, while the surface of copper can be covered by an absorbing oxide layer, significantly reducing the efficiency of surface plasmons [32]. For this reason, silver was used as the metal in this work and its optical constants were taken from [33]. WSe_2 was used as the semiconductor film since it is one of the most studied two-dimensional semiconductors and its optical constants are well known for both monolayer and multilayer samples [34]. This approach can be applied to any type of TMD with known optical constants.

Simulation of optical radiation propagation in the structure under consideration was carried out using the *COMSOL Multiphysics*[1] software package in the Wave Optics extension module. The configuration being studied contains several key parameters which

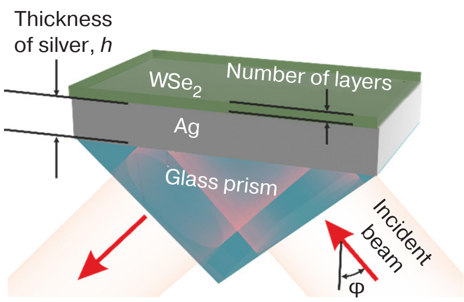

Fig. 1. Schematic diagram of the structure under study

contribute most to the simulation results. Parameters such as silver thickness and the number of TMD layers have technological limitations and can be chosen over a wide range of thicknesses. The angle of incidence of optical radiation at the metal/dielectric interface is also a variable parameter. At the same time, it is important for the Kretschmann geometry to use the transverse magnetic mode of the incident radiation. This is the necessary condition for the generation of surface plasmon waves. The wavelength of the incident optical radiation was equal to 740 nm, corresponding to the position of the exciton peak for WSe_2. Varying these parameters enables the distribution of electric and magnetic fields in the structure to be changed. This allows the parameters for the highest possible power density of optical electromagnetic radiation in the region of the two-dimensional semiconductor film to be defined.

RESULTS AND DISCUSSION

Figure 2 shows plots of the maximum absorption value as a function of the number of semiconductor film layers, the angle of light incidence, and the thickness of the silver layer. This value in this case means the maximum value among all other varying parameters.

[1] https://www.comsol.com/. Accessed June 01, 2023.

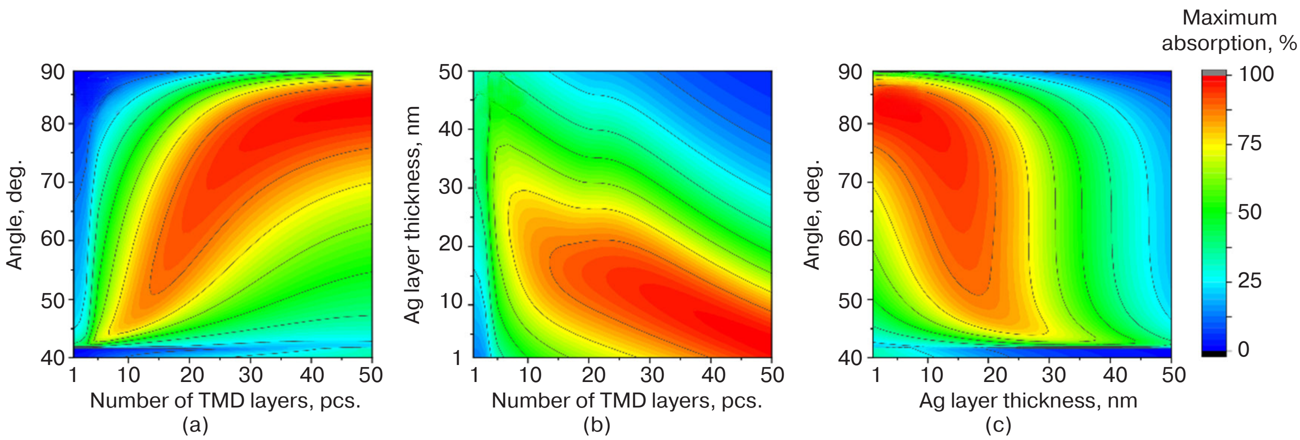

Fig. 2. Diagrams of dependence of the maximum absorption value in WSe_2 in the configuration with a homogeneous silver layer as a function of: (a) the angle of incidence of radiation and the number of TMD layers, (b) the thickness of the Ag layer and the number of TMD layers, (c) the angle of incidence of radiation and the thickness of the Ag layer

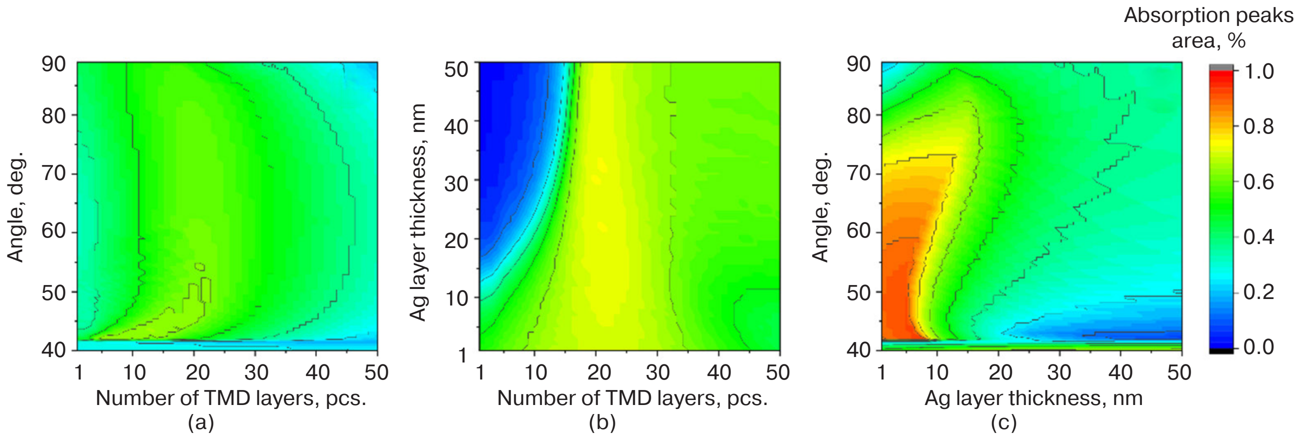

Fig. 3. Diagrams of the dependence of the area of absorption peaks in WSe_2 in the configuration with a flat silver layer as a function of: (a) the angle of incidence of radiation and the number of PDM layers, (b) the thickness of the Ag layer and the number of TMD layers, (c) the angle of incidence of incident radiation and the thickness of the Ag layer

In Fig. 2a, the maximum values for all other parameters (in this case, it is the thickness of the silver layer) are shown in the coordinates of the angle of incidence and the number of layers. The maximum absorption values for all values of the silver layer thickness were taken from among the sets of plots in the coordinates of the angle of incidence and the number of TMD layers. If the point with the maximum absorption value of 99% is taken (according to the coordinates of the number of TMD layers 40 and the angle of incidence 80°), then by any other graph (Figs. 2b and 2c) the value of the third coordinate can be defined: the thickness of the silver layer, at which this maximum value is achieved. So from Figs. 2b and 2c it is clear that this value of the silver layer thickness is ≈8 nm.

Figures 2a and 2b show that in such a configuration of the Kretschmann model, the maximum value of absorption in the TMD (close to 100%) can be achieved only with a large number of semiconductor layers (15 and more). Nevertheless, it shows that it is possible to achieve such a large percentage of absorption just in the semiconductor layer (which can be a conducting channel for optoelectronic devices), and not in the whole structure (as, for example, shown in the works analyzed in the introduction of this article).

In addition to the maximum optical absorption value, the area of the absorption peak is a characteristic value. This value must be taken into account because, for example, at different beam angles the maximum optical absorption values may be the same, while the areas of these absorption peaks may differ radically from each other. This fact can be decisive when selecting the configuration for the respective applications. Therefore, a plot of the absorption peak area as a function of the number of semiconductor film layers, the angle of light incidence, and the thickness of the silver layer was also calculated. The results of this calculation are shown in Fig. 3. The area of the peaks in this case refers to the number of points with a value above 68% (2σ, where σ is the standard deviation), of the absorption maximum. This analysis is also necessary because if the absorption peak is very narrow in some coordinates, it is technologically difficult to create a structure with such precise tolerances. It is thus important to determine not only the absorption maximum value, but also its area.

Figure 3c shows the specific parameters at which a large area of the absorption peaks is achievable. For example, it can be seen that a large area of the absorption peak is achieved with a silver layer thickness of up to 5 nm, and an angle of incidence of 42° to 60° (Fig. 2c shows that this peak roughly corresponds to an absorption value of 50%).

Figure 4 shows a diagram of the dependence of absorption in TMD on the thickness of the silver layer and the angle of incidence of light. The dotted white line in the inset shows the region with the maximum absorption value. It can be concluded that the use of monolayer TMD is not very advantageous in terms of achieving high optical absorption (Fig. 4 shows the maximum achievable absorption value of 40%). However, for nanoelectronics devices and other applications, energy-efficient semiconductors need to be used. Monolayer TMD specifically belong to this group, due to their direct bandgap. It can also be advantageous in terms of device integration and miniaturization. Hence, there is an obvious interest in finding methods to increase the name absorption in a monolayer film. It can be seen clearly from Fig. 4, that the optimal values of parameters for achieving maximum absorption in a monolayer film are: the thickness of the silver layer is 37 nm and the angle of incidence of incident radiation is 42.1°.

As mentioned above, the important quantity under study is the absorption by the semiconductor layer. In Fig. 5, the solid lines show the plots of absorption, reflection and transmittance of the whole structure as a function of the angle of incidence of light for different thicknesses of the silver layer, and the dashed line shows

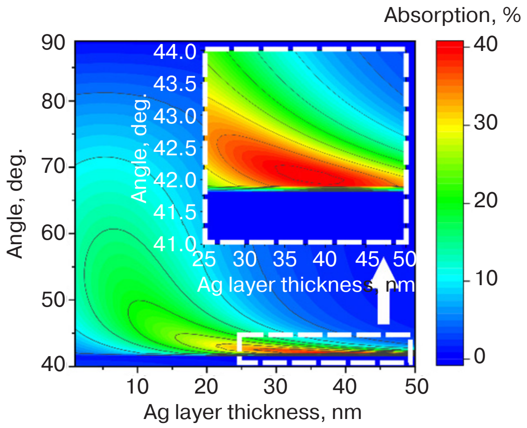

Fig. 4. Diagram of the absorption dependence in TMD as a function of the silver layer thickness and the angle of light incidence

the plots of absorption of as a function the semiconductor layer. These are typical plots that arise when using the Kretschmann geometry [35].

The width of the absorption peaks indicates the increase of absorption exactly due to plasmon resonance. Figure 5d shows a plot of the magnetic field distribution (H_z-component) in a structure with a silver thickness of 37 nm and a light incidence angle of 41.2°, i.e., the peak of plasmon resonance and absorption in Fig. 4. Here standing waves can be seen, the appearance of which is characteristic of surface plasmon resonance. It can also be seen that in this case, the absorption in the semiconductor film is only half of the total absorption of the structure.

Figure 6a shows the absorption map of the total structure as a function of silver layer thickness and

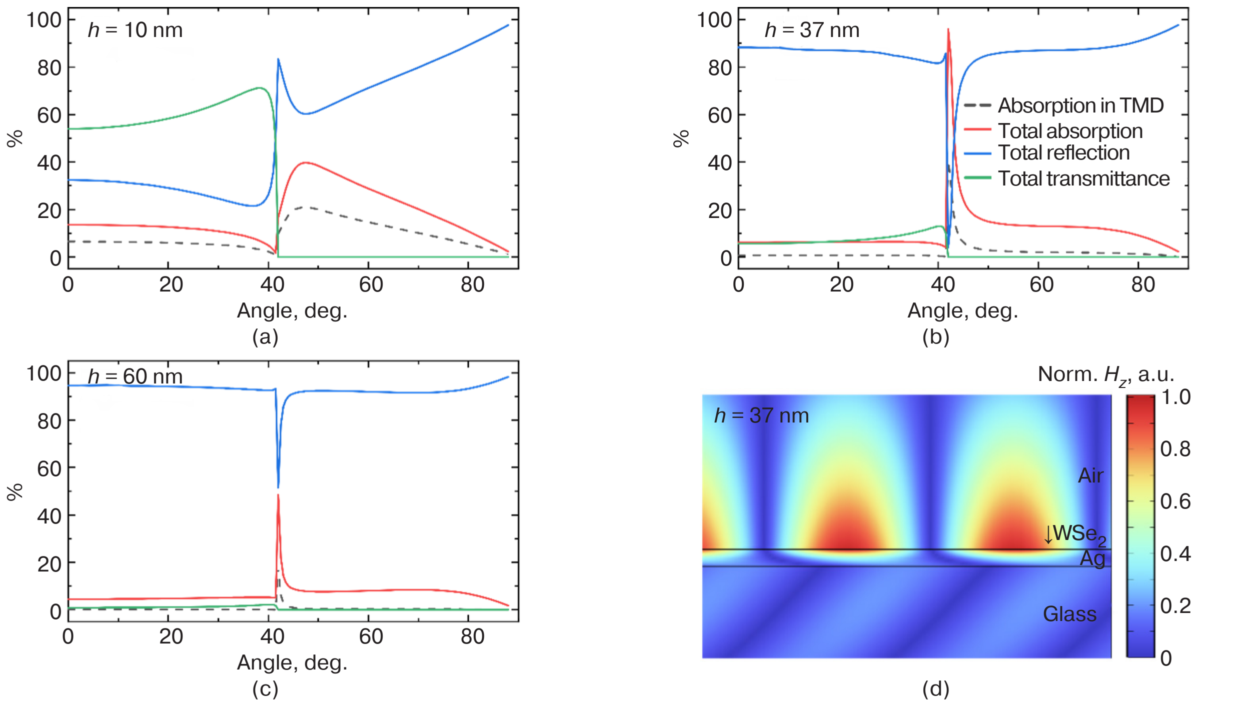

Fig. 5. Diagrams of absorption, reflection and transmittance as a function of the angle of incidence of light for structures with silver layer thicknesses of 10 (a), 37 (b), and 60 (c) nm and normalized graph (d) of magnetic field (H_z-component)

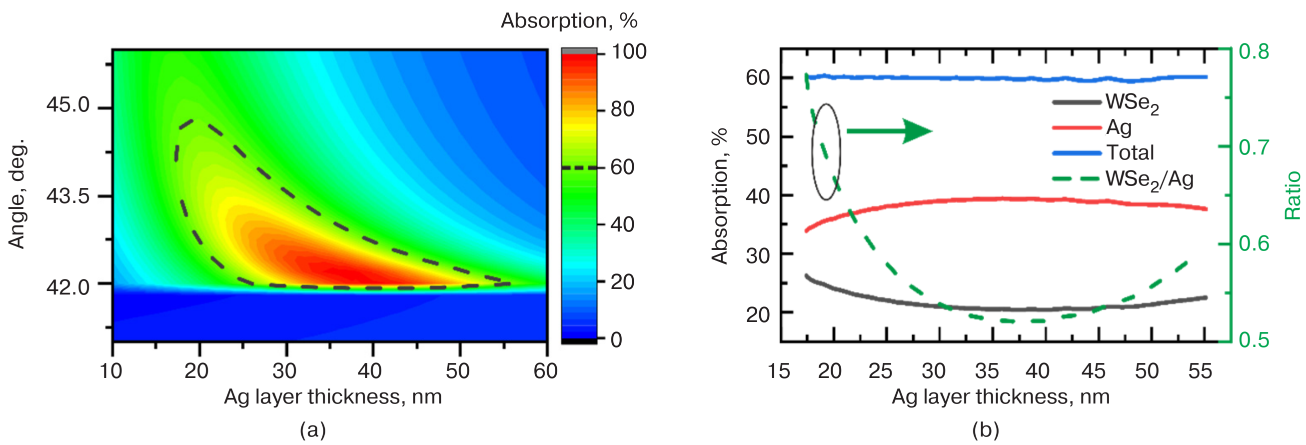

Fig. 6. Optical absorption map in the total structure as a function of silver layer thickness and beam angle of incidence (a) calculated absorption values in WSe_2 and Ag film separately as a function of Ag layer thickness (b)

angle of incidence (WSe_2 thickness is one monolayer). The contour of the graph with an absorption level of 60% (black dashed contour) was chosen as an example. As can be seen from the graph, an overall absorption equal to or greater than 60% can be achieved using different combinations of metal thickness and angle of incidence. However, this does not mean that the absorption in the TMD will be maximized. In order to demonstrate this effect, the absorption in the monolayer film, silver, was further calculated along the white line with arrows and the ratio of these absorptions was calculated (black, red, and dashed green lines in Fig. 6b). It can be clearly seen that the absorption of the total structure is 60% in the entire graph, but the absorption plots of the individual layers of the structure are not constant. The dotted green graph shows that the ratio of absorption in the semiconductor to absorption in the metal can vary from 0.7 to 0.5, i.e., differ almost by a factor of 1.5.

CONCLUSIONS

In the framework of this work, a theoretical study of optical absorption in a semiconductor WSe_2 film with Kretschmann configuration was conducted. The study took into account such parameters as the thickness of WSe_2, the thickness of the silver layer and the angle of light incidence. At the exciton peak wavelength (740 nm), a high absorption level (more than 80%) is achieved when the thickness of WSe_2 is 8 nm and above (corresponding to 15 monoatomic layers). In this case, the thickness of the silver layer is up to 20 nm and the angle of incidence in the range of 50° to 85°. In order to achieve 100% absorption, a WSe_2 thickness of about 22 nm or more (corresponding to 40 layers) is required. The Ag layer thickness value should be less than 10 nm, and the angle of incidence in the range of 55° to 85°.

The maximum achievable "area" of the absorption peak is observed at a silver layer thickness of up to 5 nm and an angle of incidence between 42° and 60°. For monolayer film, the optimum absorption values are achieved at a silver layer thickness of 37 nm and an incidence angle of 42.1°. Under these conditions, the total absorption in the structure is 100%, whereas the absorption in the monolayer film is 40%.

The importance of determining the optimal parameters for absorption directly in the semiconductor film needs to be emphasized. Despite the same absorption values throughout the structure, the absorption ratio between the WSe_2 semiconductor layer and the Ag metal layer can vary between 0.7 and 0.5. This information is of key importance for the development of nano- and optoelectronics devices such as phototransistors and photodetectors with a two-dimensional semiconductor channel.

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Authors' contributions

A.A. Guskov—theoretical modeling, conducting numerical calculations using the finite element method to solve Maxwell's equations, and writing the text of the article.

N.V. Bezvikonnyi—visualization and systematization of results, creating graphs and diagrams illustrating key parameters and the dependence of light absorption efficiency on various factors.

S.D. Lavrov—overall project supervision, formulation of the research problem, strategic direction of the project, ensuring the achievement of set goals and high quality of the results.

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