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Absorption Enhancement for Black Phosphorus Active Layer Based on Plasmonic Nanocavity

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Abstract: In this letter, we propose a strategy to enhance absorption in the black phosphorus absorber based on a nanocavity structure. By introducing a porous silver layer, an enhanced broadband light absorption can be obtained in the spectral range of 520–820 nm. The optical characteristics of the black phosphorus absorptive layer are thoroughly analyzed by absorption spectra, electric intensity distribution, and power flow distribution. Numerical and analytical analysis revealed that the optical absorption of the black phosphorus layer with a porous silver layer can be enhanced by 50% and 396% at the resonant wavelength of 690 nm for p-polarized and s-polarized incidences, respectively, when compared to that without a silver layer. Furthermore, the short-circuit current density ($J_{SC}$) was calculated for the proposed architecture. The peak value of $J_{SC}$ was more than 18 mA/cm². It is demonstrated that this super absorption structure could find important applications on plasmonic-assisted photovoltaic devices or other opto-electronic devices, which will promote the development of ultrathin-on-chip energy harvesting and new thin-film active devices.

Index Terms: Black phosphorus, porous silver layer

1. Introduction

Recently, photovoltaic (PV) technology has attracted a great concern due to the capability of providing an unlimited source of clean energy by efficiently converting energy of light into electricity. New design approaches and materials need be investigated to make high-efficient solar cells a decent alternative to fossil fuels. Solar cells can be usually classified into first, second and third generation cells. Solar cells with a number of thin-film technologies and many novel materials are described as the third generation solar cells. Despite the fact that the third generation solar cells have not yet been widely used and are even still in the research, thin-film technologies have found an increasingly wide utilization in producing low-cost, high-efficient solar cells. Absorption enhancement strategies should be introduced into ultrathin-film devices due to the fact that there is a long-existing trade-off between optical absorption and the thickness of the absorptive layer, which are highly desirable for a broad range of energy applications including thin-film photovoltaics [1]–[3]. Until now, most of the solar cells are based on the mechanism of nanocavity. The principle
of the nanocavity is using cavity to limit the photon, producing resonance to enhance the absorptive energy with the back and forth reflection of light [4]. In conventional optoelectronics investigation, resonant cavity mechanism has been widely used to enhance the performance of photonic devices, including photodetectors [5], light emitting diodes [6], phototransistors, modulators, wavelength division multiplexing systems [7], etc. Simultaneously, several other light trapping strategies have been proposed, including folded configurations [8], diffraction gratings [9], direct coupled resonators [10], and plasmonic nanostructures [11]–[22]. Among these approaches, the use of plasmonic nanostructures for light enhancement is quite promising, which can realize compact plasmonic devices and circuits [23]–[25]. Surface plasmon polaritons (SPPs) are electromagnetic excitations coupled to electron oscillations that propagate along metal-dielectric interface and their field amplitudes decrease exponentially perpendicular to the interface, resulting in a strong subwavelength optical confinement [26]. More importantly, it breaks through the optical diffraction limit and enhances absorptive energy. Nanocavity based on SPPs can combine the properties of SPPs with nanocavity’s characteristic, which develops a new strategy to realize absorption enhancement for various ultra-thin absorptive materials.

Two-dimensional (2D) material monolayers are promising candidates to be employed as the absorptive layers for atomically thin energy harvesting devices [27]. The recent isolation of atomically thin black phosphorus by mechanical exfoliation of bulk layered crystals has triggered an unprecedented interest. The bandgap of black phosphorus is tunable in the range of 0.3-2 eV [28]–[30], which is a very appealing feature as the band gap value spans over a wide energy range. Importantly, it has recently attracted intensive interests in optoelectronics attributed to the strong light absorption leveraged on the presence of direct band gap, which is potential for the use of photovoltaic energy harvesting and photocatalysis applications. So exploring the absorption enhancement for black phosphorus active layer based on SPPs-nanocavity is significant.

In this paper, we employ a porous silver layer to enhance the optical absorption in the black phosphorus active layer. Optical characteristics of the porous structure are thoroughly analyzed by absorption spectrum, optical field intensity and power flow. Numerical modeling results show that this absorber can realize super absorption. Further, the short circuit current density \( J_{SC} \) was calculated to evaluate the performance of this PV device. This super absorption structure is particularly promising for the development of ultra-thin on-chip energy harvesting and conversion applications.

2. Numerical Simulation of the Porous Nanocavity
As illustrated in Fig. 1, the proposed porous structure consists of an Al metal reflector, an \( \text{Al}_2\text{O}_3 \) lossless layer, a black phosphorus absorptive layer and a silver film patterned with a periodic
nanohole array. The metal reflector is set to be 100 nm to eliminate the optical transmission. Consequently, the total absorption, $A(\lambda)$, can be expressed as $A(\lambda) = 1 - R(\lambda)$, where $R(\lambda)$ is the reflection. The previous investigations on the mechanism of the resonant absorption found that the key issue in the two-layered system is that the light can penetrate into the metal reflector and lead to a large phase change, which will result in optical loss in the metal film. Therefore, an $\text{Al}_2\text{O}_3$ lossless layer is introduced between the absorptive layer and the metal reflector, which can reduce the total reflection and enhance the absorption of the black phosphorus layer by compensating the phase mismatch [31]. A schematic diagram of the black phosphorus crystal structure is shown in the inset of Fig. 1. This atomic arrangement yields two inequivalent directions within the black phosphorus lattice: the zigzag and the armchair, leading to its unusual in-plane anisotropic electrical and optical properties. A porous silver layer is covered on the top of the black absorptive layer due to the capability of supporting SPPs, which yields strong confinement of optical fields over a broad spectral range. To determine the optical absorption property, here we employ the finite element method (FEM) to model the absorption spectra of the porous structure. The optical constants of Ag, Al, and $\text{Al}_2\text{O}_3$ are extracted from ref. [32]. Real and imaginary parts of the refractive index of the black phosphorus are the functions of wavelength [33], the refractive indices of black phosphorus film were characterized by the interpolation function of the wavelength in our simulation. For instance, we used the complex refractive index ($n_{\text{AC}} = 2.65 + 0.595i, n_{\text{ZZ}} = 2.69 + 0.25i$) around the wavelength of 520 nm. The geometric parameters of the structure (i.e., the period, $P$, the diameter of the nanohole, $D$, the thickness of the porous Ag layer, $t_{\text{Ag}}$ and the thickness of the $\text{Al}_2\text{O}_3$ lossless layer, $t_{\text{Alumina}}$) are systematically optimized to realize super absorption. Moreover, the absorption in the porous silver layer will not contribute to the energy conversion, so we calculated absorption contributed by metal ($A_{\text{metal}}(\lambda)$) and analyzed the exclusive absorption in the black phosphorus in our simulation.

According to the previous report [34], introducing a lossless layer in a planar cavity structure can maximize the absorption in the active layer. Consequently, we first focus on the impact of the $\text{Al}_2\text{O}_3$ lossless layer thickness on the absorption spectra. As shown in Fig. 2(a), the absorption in the
active layer for six different thicknesses are plotted, showing a strong dependence of the resonance wavelength on $t_{\text{Alumina}}$. The resonant condition of this system can therefore be controlled with a wider tunability. Importantly, the absorption can be enhanced with the adjustment of $t_{\text{Alumina}}$. For instance, as shown by the pink and black solid line in Fig. 2(a), the peak absorption of the absorptive layer was enhanced to 63% at 580 nm. To demonstrate the effect of $t_{\text{Alumina}}$ on the absorption, we modeled the absorption spectra as the function of the Al$_2$O$_3$ lossless layer thickness under the illumination of p-polarized [see Fig. 2(b)] and s-polarized states [see Fig. 2(c)], respectively. For the p-polarized incidence as shown in Fig. 2(b), the absorption peak above 80% can cover a wavelength range of 548–800 nm, the peak total absorption value even grows to 91.3% at 620 nm, when $t_{\text{Alumina}}$ is 50 nm. For the s-polarization case as shown in Fig. 2(c), one can see that a similar enhanced and $t_{\text{Alumina}}$-sensitive absorption resonance can also be obtained. Compared to Fig. 2(b), the absorption enhancement has declined, especially in the spectral region of 600–740 nm. To reveal the power flow in the nanocavity, the spatial Poynting vector distribution is shown in Fig. 2(d). One can see that the amplitude of the Poynting vector decreases significantly through the 30-nm-thick black phosphorus layer, indicating the strong absorption in this 30-nm-thick absorptive layer. Therefore, the thickness of the lossless layer was set to 50 nm to achieve super absorption under normal incidence.

Next, to better analyze the influence of the porous silver layer thickness on the optical characteristics, the absorption spectrum is modeled as the function of the thickness $t_{\text{Ag}}$ as depicted in Fig. 3(a) and (b). Two polarized state incidences were employed to explore the absorption spectra of the structure. The spectral absorption varies with the thickness $t_{\text{Ag}}$. While the optical absorption enhancement varies with the thickness of the porous silver layer, a large enhancement can be observed over a broad spectral range from 550 nm to 820 nm for $t_{\text{Ag}}$ between 5 nm and 15 nm shown in Fig. 3(a). The bandwidth of the absorption enhancement becomes wider and the width of the enhancement spectrum at the thickness of 10 nm is approximately 5 times broader than that at $t_{\text{Ag}} = 100$ nm. The absorption spectrum for s-polarized incidence is plotted in Fig. 3(b), in contrast to that shown in Fig. 3(a). One can see that a similar enhanced and $t_{\text{Ag}}$-dependence absorption resonance can also be obtained. A super absorption can be observed over a broad spectral range from 550 to 800 nm for $t_{\text{Ag}}$ in the range of 10–25 nm, which is a little broader than that for p-polarized incidence. In addition, a strong absorption peak is obtained at $t_{\text{Ag}} = 21$ nm, which is different from that obtained (i.e., 7 nm) for p-polarized incidence. To verify this absorption enhancement, the electric field distribution at a wavelength of 800 nm for p-polarized incidence was calculated and plotted in Fig. 4(a)–(d). Fig. 4(a) and (b) respectively show the electric field distribution at top and bottom of the nanohole in X-Y plane, which illustrates that the SPPs mode is mainly concentrated in the space around the single hole of periodic units. In X-Z plane shown in Fig. 4(c), the SPPs mode is concentrated near the Ag/black phosphorus interface and air/Ag interface. Due to the fact that p-polarized incidence should not excite any plasmonic mode in Y-Z plane, Fig. 4(d) only shows a normal reflection interference pattern. This resonance should be attributed to the excitation of SPPs modes. To effectively trap light in the black phosphorus layer, it proposes a strategy to enhance
the optical absorption of the black phosphorus layer based on strong SPPs modes at the Ag/black phosphorus interface. According to Fig. 3(a) and (b), the $t_{Ag}$ was selected at 10 nm to achieve absorption enhancement of the structure over a wide range of incident wavelength.

To further interpret the effect of the thickness on the SPPs modes excitation at the Ag/black phosphorus interface, the spatial distribution of the electric field at four different thicknesses of the porous silver layer is revealed in Fig. 5(a)–(d). It can be observed the electric intensity is enhanced as $t_{Ag}$ decreases. We focus on the electric intensity at Ag/black phosphorus interface,
which shows that the electric intensity confined around Ag/black phosphorus interface at $t_{Ag} = 10$ nm is almost 3 times larger than that at $t_{Ag} = 100$ nm. Comparing the surface charge density on the top and bottom of the porous silver layer at $t_{Ag} = 10$ nm as shown in Fig. 5(e), it clearly has a symmetric charge density distribution showing that the mode excited at the interface is the short-range SPPs (SRSPPs) mode [35], [36]. As shown in Figs. 3 and 5, when the thickness decreases from 100 nm to 5 nm, the modes turn into SRSPPs mode gradually, with an obvious enhanced optical absorption over 80% in a broad range of incidence. In addition, from Fig. 3(a) and (b), it is found that the bandwidth of the absorption enhancement spectra becomes wider when the modes turn into SRSPPs. In short, the total absorption is much higher and spectrally broader for smaller thicknesses. Based on the modeling results, it is believed that the proposed porous silver layer can not only enhance the absorption but also broaden the absorption enhancement spectrum. From the discussion above, $t_{Ag}$ was determined to be 10 nm by comparing absorption spectra of p-polarized and s-polarized incidences, respectively.

As presented before, the optical properties of SRSPPs supported by ultra-thin nanoporous silver layer can be tuned by varying the geometry parameters. We discuss the tunability of the nanohole array (i.e., the period, $P$, the diameter of the nanohole, $D$) of the multi-layer structure. For simplicity, one parameter was kept constant and the other varied in these simulations. We first consider tuning $D$ in an ultra-thin porous silver layer. The spectrum of the absorption as a function of wavelength and the diameter $D$ is shown in Fig. 6(a) ($P = 300$ nm), which shows that although the spectral absorption varies with the diameter $D$, a high absorption is observed (e.g., > 0.7, with a peak value of ~1) over a broad spectral range from 550 to 820 nm for $D$ in the range of 160–250 nm. One can see that the absorption at $D = 170$ nm is broader than other diameters. Next, we discuss the tunability of the $P$. Fig. 6(b) shows 2D map of the optical absorption enhancement as a function of the incident wavelength and nanohole array period ($P$), while other structural parameters are kept constants ($D = 170$ nm). Three distinct shifts of the absorption peak can be observed in three spectral ranges when $P$ is tuned from 200 to 600 nm. When the spectra region lies in the ranges of 520–600 nm and 680–820 nm, the absorption peak red-shifted. When the wavelength increases from 600 to 680 nm, the absorption peak blue-shifted. The resonance mode in the spectral region...
Fig. 7. The absorption spectra of the three structures for (a) p-polarized and (b) s-polarized incidences, respectively. Black line - the absorption spectrum with a porous silver layer structure of the diameter $D = 170$ nm, and the period $P = 300$ nm; red line – the absorption spectrum with a flat silver layer structure; blue line – the absorption spectrum without a silver layer.

of 600–680 nm approaches to the other two and finally forms a single mode at $P = 230$ nm and $P = 550$ nm, respectively. An interesting trend can be identified in Fig. 6(a) and (b): the red-shift shown in Fig. 6(a) has an opposite trend to that in Fig. 6(b). To further reveal the spectral tunability of the nanohole array, we modeled the optical absorption of the total structure by optimizing $D$, where the period/diameter ratio was kept as a constant. It can be seen in Fig. 6(c)–(e) that the period/diameter ratio played an important role to enhance the absorption. One can see clearly from Fig. 6(c) that resonant wavelength mainly covers three spectra ranges. Compared to Fig. 6(c), the absorption enhancement spectra became broader when the period/diameter ratio was set as 1.76 [see Fig. 6(d)]. As shown in Fig. 6(e), when the period/diameter ratio was set to 2, one can see that the absorption is not only a little lower but much narrower than the other two. In summary, according to the absorption spectra shown in Fig. 6(a)–(e), the period $P$ was set to be 300 nm and the diameter $D = 170$ nm.

By numerically designing the geometric parameters of the thickness $t_{\text{Ag}}$, $t_{\text{Alumina}}$, the period $P$, and the diameter $D$, the perfect absorption can be freely tunable. Fig. 7(a) and (b) give the optical absorption spectra for the porous nanocavity with the optimized geometric parameters. As shown in Fig. 7(a), the absorption spectra for the structure with a porous silver layer (black line), a flat silver layer (red line) and the one without a silver layer (blue line) are plotted for p-polarized incidence. It can be observed that absorption enhancement of the porous structure is significant in the two spectral regions (554–644 nm and 706–820 nm) compared to the flat silver structure. In general, the absorption over 80% can cover a spectra range from 548 nm to 800 nm. As for the structure without a silver layer, it shows the strong dependence of the absorption on wavelength (see blue line), which means that it is not suitable applied in the energy harvesting application. Fig. 7(b) describes the absorption spectra of the structures for s-polarized incidence. It can be clearly seen that in the short wavelength side ($\lambda < 560$ nm), the absorption of the structure with a porous silver layer (see black line) is a little lower than that of the structure with a flat silver layer (see red line). However, the absorption is obviously stronger in the long wavelength side. For the structure without a silver layer (see blue line), the absorption is significantly suppressed when compared to that with a porous layer. Compared to the other structures, the proposed porous structure (with optimal structural parameters, $P = 300$ nm, $D = 170$ nm, $t_{\text{Ag}} = 10$ nm, and $t_{\text{Alumina}} = 50$ nm) exhibits an improved performance due to the excitation of SRSPPs modes, especially for s-polarized incidence. The proposed plasmonic nanostructure can concentrate the energy into the absorptive layer, leading to the enhanced absorption and it can also be found that absorption peak become more steady which can support a broadband light absorption. The calculations show that compared with a no silver structure, an optimized porous plasmonic structure can enhance the absorption by 50% and 396% for p-polarized and s-polarized incidences, respectively. It suggests that this porous nanostructure strategy would be also beneficial for the photovoltaics with other 2D materials.

Since the absorption is dependent on incident angles, we then analyze the dependence on this parameter. As shown in Fig. 8(a), when we employ a p-polarized incidence to illuminate the
multi-layer system with optimized geometric parameters (i.e., \( P = 300 \text{ nm} \), \( D = 170 \text{ nm} \), \( t_{\text{Ag}} = 10 \text{ nm} \), and \( t_{\text{Alumina}} = 50 \text{ nm} \)), an absorption peak over 92% at the wavelength of 620 nm is obtained at 20° of the incident angle, with a strong absorption band of black phosphorus up to 50° in the range of 550–800 nm. With the proposed structure, an omnidirectional absorption can be achieved over a wide range of incident angles. It should be noted that when the incident angle continues to increase (i.e., larger than 70°), the absorption begins to decrease rapidly and even becomes lower than 20%. For comparison, we model the angular-dependent absorption spectrum for an s-polarized incidence as shown in Fig. 8(b). It can be observed that the absorption increases along the incident angle up to 60° in the spectral range of 520–820 nm. In addition, one can clearly see that the absorption enhancement at large incident angles can be more than 50%, which is much larger than that under a p-polarized incidence. Over all, the angle-insensitive is more visible under s-polarized incidence for the fact that the absorption enhancement are all over 50%, which can be speculated that for p-polarized incidence, the transverse electric component is continuously varying with the increasing incident angle; while for the s-polarized state, its direction is always parallel to the surface. In general, the proposed strategy can realize an omnidirectional absorption up to 50° of almost all the incident angles, indicating the potential to realize the high-performance PV devices.

### 3. Analytical Analysis and Calculation

Finally, we evaluate the performance of the proposed design applied in the photovoltaic device under the solar irradiance for the standard AM1.5 spectrum \( S(\lambda) \). The absorbed photon flux density for the photovoltaic device is given by \( \phi(\lambda) = A(\lambda)S(\lambda)/E(\lambda) \), where \( E(\lambda) = hc/\lambda \) denotes the energy of a single photon. Due to the fact that the photogating effect is pronounced at the interface between black phosphorus and other materials [33], which can make it become a reality that one incident photon effectively contributes several carriers, we finally assume that every absorbed photon generates one exciton, which dissociates into holes and electrons, and all photo-induced charge carriers are collected by the electrodes. Consequently, the \( J_{\text{SC}} \) can be estimated using \( J_{\text{SC}} = e \cdot \int \phi(\lambda) d\lambda \). In the simulation, the thickness \( t_{\text{Ag}} \) of the metal film was increased from 5 nm to 100 nm. To demonstrate the achievable enhancement, \( J_{\text{SC}} \) of the cell was calculated as a function of the \( t_{\text{Ag}} \) as shown in Fig. 9. As depicted in Fig. 9, the peak value of \( J_{\text{SC}} \) was found to be 18 mA/cm² at an optimal \( t_{\text{Ag}} \) of 7 nm under p-polarized incidence (see black line). The \( J_{\text{SC}} \) of the device calculated for s-polarized incidence is displayed in Fig. 9 (see red line), which shows the value of \( J_{\text{SC}} \) can be held at around 16 mA/cm² of the \( t_{\text{Ag}} \) from 13 nm to 23 nm. Importantly, it should also be noted that both the trends of the \( J_{\text{SC}} \) are to rise first and then fall, which corresponds to the red-shift shown in Fig. 3. With the change of the \( t_{\text{Ag}} \), the absorption peak was at 7 nm and 20 nm as shown in Fig. 3(a) and (b), respectively. Above all, the absorption has a great impact on the \( J_{\text{SC}} \), the geometry parameters of the porous silver layer need to be selected to achieve the maximum absorption. The design principle of the nanopatterned metallic structure proposed in this article can be incorporated...
into photovoltaic devices, which offers a promising approach to improve performance of ultra-thin energy harvesting devices.

4. Conclusion
In conclusion, the design of a black phosphorus absorptive layer based on plasmonic nanocavity is proposed. By properly designing the geometric parameters of the structure, the optical absorption of the black phosphorus layer can be enhanced significantly. We presented a systematic investigation on the effect of absorption enhancement mechanism at black phosphorus absorptive layer by absorption spectrum, electric field distribution and power flow. Numerical modeling results show that absorption is enhanced by introducing SRSPPs modes. Compared to no silver absorber, the total absorption of the porous absorber with the optimized geometric parameters was found to be enhanced by as much as 50% and 396% at the resonant wavelength for p-polarized and s-polarized incidences, respectively. What's more, the calculations show that the $J_{SC}$ of the cell can be more than 18 mA/cm$^2$ when the thickness $t_{Ag}$ was suitably selected. This structure can improve the performance of the organic solar cells. Importantly, this design strategy can also be employed for other 2D materials and multi-layer structure, which will pave the way towards highly efficient ultra-thin materials with enhanced by introducing light-matter interactions for energy harvesting applications and promote the development of novel thin-film active devices.

References


