Control of absorption of monolayer MoS$_2$ thin-film transistor in one-dimensional defective photonic crystal

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received 20 August 2015; accepted in final form 2 November 2015; published online 26 November 2015

PACS 78.67.-n – Optical properties of low-dimensional, mesoscopic, and nanoscale materials and structures
PACS 42.25.Bs – Wave propagation, transmission and absorption
PACS 85.60.Jb – Light-emitting devices

Abstract – The light absorption and transmission of monolayer MoS$_2$ in a flexible one-dimensional defective photonic crystal (d-1DPC) are theoretically investigated. The study shows that the strong interference effect decreases the photon density in particular areas of the microcavity. The d-1DPC can reduce light absorption of the monolayer MoS$_2$ and enhance light transmission. The impact of monolayer MoS$_2$ light absorption on the localization effect of the photon is investigated when the monolayer MoS$_2$ and the organic light-emitting diode are located in the same microcavity. However, monolayer MoS$_2$ does not reduce the emission intensity from the microcavity by regulating the position of monolayer MoS$_2$ in the microcavity.

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A transparent and flexible thin-film transistor (TFT) is the foundation of next-generation display technology. Traditional transparent and flexible TFT is mostly based on oxide semiconductors, organic materials, and carbon nanotubes [1–3]. Recently, monolayer MoS$_2$ TFT has elicited considerable attention [4]. Monolayer MoS$_2$ exhibits good electrical and mechanical properties. TFT made of monolayer MoS$_2$ consume very low power with high on/off ratio up to $10^5$ [5–10], which is significantly higher than that of graphene TFT [11]. Given its excellent flexibility, the electrical property of monolayer MoS$_2$ TFT slightly changes even after bending to a curvature radius of 0.75 mm for hundreds of times [5].

However, monolayer MoS$_2$ shows higher light absorption ($\sim$10%) [1,2,12–14]. The transmittance of monolayer MoS$_2$ is only 70% to 90%. Monolayer MoS$_2$ is an efficient material for photoelectric detectors. Its conductivity is very sensitive to light [12]. The photoresponsivity of monolayer MoS$_2$ can reach 880 A/W. Thus, the backlight absorption of monolayer MoS$_2$ affects its conductivity, thereby decreasing the on/off ratio. These features are unfavorable for creating transparent monolayer MoS$_2$ TFT with light irradiation. Transparent TFT can extend the application scope of display technology, increase the opening ratio of display elements, and reduce power consumption.

Therefore, light absorption and transmission should be regulated for creating transparent monolayer MoS$_2$ film transistors. Many researchers have investigated the optical regulation of graphene and monolayer MoS$_2$. Previous studies mostly focused on different optical microstructures to enhance the absorption of two-dimensional materials [15–30]. For example, the one-dimensional defective photonic crystal (d-1DPC) microcavity can be used to significantly enhance two-dimensional materials absorption due to the localization effect of light in microcavity [16–20]. This enhancement is mostly based on the strong interference effect of light. Light interference can usually enhance the absorption in particular areas and reduce their absorption in other areas [31]. Therefore, d-1DPC can be used similarly to reduce the absorption of...
two-dimensional materials. The commercial flexible photonic crystal production process is very mature today [32]. As such, composite structures composed of flexible 1DPC and monolayer MoS2 are expected to exhibit excellent mechanical properties.

In this paper, the regulatory function of d-1DPC on the light absorption and transmission of monolayer MoS2 is investigated theoretically. In d-1DPC, 20–30 times of monolayer MoS2 light absorption can be reduced. Its transmission can also reach up to 98% and above. However, in d-1DPC, light absorption and transmission of monolayer MoS2 are sensitive to the thickness of defective layer and incident angle. To overcome this weakness, we examined the emission intensity from the microcavity when monolayer MoS2 and microcavity organic light-emitting diodes (OLED) [32–36] are located in the same microcavity. After regulating the position of monolayer MoS2 in the microcavity, monolayer MoS2 did not reduce emission intensity from the microcavity. Integration of monolayer MoS2 and OLED can significantly overcome the above-mentioned weakness, reduce the pixel size, and improve the opening ratio of TFT.

The detailed structure is shown in Fig. 1(a). The d-1DPC is formed by the (AB)\textsuperscript{M1} ACMCGA(BA)\textsuperscript{M2} structure, where A and B refer to the two different kinds of transparent organic films. Their refractive indexes are 1.7 (polyimides) and 1.5 (poly(methyl methacrylate)) [37], respectively. TheSC layer is a kind of transparent organic film with a refractive index of 1.5. M and G refer to monolayer MoS2 and graphene layer, respectively. The two C layers, monolayer MoS2, and graphene layer constitute the defective layer. Monolayer MoS2, graphene layer and one of the C layers constitute the flexible TFT [8]. The thickness of the monolayer graphene and monolayer MoS2 is \( d_g = 0.34 \text{ nm} \) and \( d_{MoS2} = 0.65 \text{ nm} \), respectively. The refraction index of graphene layers in the visible range is \( n_g = 3.0 + c_1 \sqrt{2} z \), where \( c_1 = 5.446 \text{ \mu m}^{-1} \) [38]. In the calculation of optical absorption, the optical conductivity of graphene can be used, which can avoid using a three-dimensional dielectric function and also shows high numerical precision [39]. For MoS2, to show the physical mechanism of the exciton optical transition and band optical transition directly, the relative permittivity is presented. The permittivity of monolayer MoS2 can be extracted from the experiments through the use of two exciton and band transitions [13,40]. The transverse imaginary permittivity of monolayer MoS2 can be given by [13,40]

\[
\varepsilon_i(\omega) = \frac{f^{A}_{ex} \Gamma_A}{(\varepsilon_{\omega} - E^2_{ex})^2 + \Gamma_A^2} + \frac{f^{B}_{ex} \Gamma_B}{(\varepsilon_{\omega} - E^2_{ex})^2 + \Gamma_B^2} + \frac{f^{A}_{ex} \Gamma_A}{E_{\omega} - E^2_{ex} + i \varepsilon_i} \varepsilon_i E_{\omega} - E^2_{ex} + \Gamma_B^2 \varepsilon_i),
\]

where \( e \) is the electron charge, \( h \) is the reduced Planck constant, the linewidth of A (B) excitons is \( \Gamma_A = 28 \text{ meV} \) (\( \Gamma_B = 48 \text{ meV} \)), the equivalent oscillator strength of A (B) excitons is \( f^{A}_{ex} = 0.32 \text{ eV} \) (\( f^{B}_{ex} = 0.43 \text{ eV} \)), the transition energy of A (B) excitons is \( E^A_{ex} = 1.884 \text{ eV} \) (\( E^B_{ex} = 2.02 \text{ eV} \)), \( E^A_{\omega} = 2.43 \text{ eV} \) is the band gap, \( E_{\omega} \) is photon energy, \( f_{\gamma} = 59 \) is the equivalent oscillator strength of interband transition, \( \Theta(x, \gamma) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f}{\varepsilon_i^2} \text{d} \varepsilon_i \) is the step function with a broadening of \( \Gamma \), while \( \Gamma_{\text{band}} = 0.398 \text{ eV} \) is the linewidth of the interband transition. The real part of the permittivity of monolayer MoS2 can be obtained using Kramers-Kronig relations

\[
\varepsilon_{\omega} = \frac{4\pi}{c} \int_{-\infty}^{\infty} \frac{\gamma}{\varepsilon_i^2} \text{d} \varepsilon_i,
\]

where \( \gamma = \frac{1}{2} \text{Re} \varepsilon_i \). For MoS2, the optical conductivity can be used, which can avoid using a three-dimensional dielectric function and also shows high numerical precision [39].

The transfer-matrix method was used for the calculation [40,41]. In the l-th layer, the electric field of the TE mode light with incident angle \( \theta_i \) is given by

\[
E_l(z, y) = A_l e^{ik_{\text{ex}}(z-z_l)} + B_l e^{-ik_{\text{ex}}(z-z_l)} e^{i k_{\text{ex}} y} e_x,
\]

and the magnetic field of the TM mode is given by

\[
H_l(z, y) = A_l e^{ik_{\text{ex}}(z-z_l)} + B_l e^{-ik_{\text{ex}}(z-z_l)} e^{i k_{\text{ex}} y} e_x,
\]

where \( k_{\text{ex}} = k_{il} + i k_{\text{h}} \) is the wave vector of the light, \( e_x \) is the unit vector in the x-direction, and \( z_l \) is the position of the l-th layer in the z-direction. The electric fields of the TE mode or the magnetic fields of the TM mode in the (\( l + 1 \))-th layer are related to the incident fields by the transfer matrix utilizing the boundary condition [40,41]

\[
\begin{pmatrix}
A_{l+1}
\end{pmatrix} =
\begin{pmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{pmatrix}
\begin{pmatrix}
A_l
B_{l+1}
\end{pmatrix},
\]

and

\[
\begin{pmatrix}
B_{l+1}
\end{pmatrix} =
\begin{pmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{pmatrix}
\begin{pmatrix}
A_l
B_{l+1}
\end{pmatrix},
\]

and

\[
\begin{pmatrix}
A_{l+1}
B_{l+1}
\end{pmatrix} =
\begin{pmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{pmatrix}
\begin{pmatrix}
A_l
B_{l+1}
\end{pmatrix},
\]

Thus, we can obtain the absorbance of the l-th layer \( A_l \) using the Poynting vector \( S = E \times H \) [40,41],

\[
A_l = |S_{(l+1)-i} + S_{(l+1)-o} - S_{(l-1)-o} - S_{(l-1)-o}| / |S_{0}|,\]

where \( S_{(l+1)-i} \) and \( S_{(l+1)-o} \) are the incident and outgoing Poynting vectors in the (\( l + 1 \))-th (\( l + 1 \))-th layer, respectively, \( S_{0} = \beta_0 A_0^2 \cos \theta_0 \) is the incident Poynting vector in air, \( S_{(l+1)-o} = \beta_{l+1} A^2_{l+1} \begin{pmatrix} \cos \theta_{l+1} \end{pmatrix} \), \( S_{(l+1)-o} = \beta_{l+1} A^2_{l+1} \begin{pmatrix} \cos \theta_{l+1} \end{pmatrix} \), \( S_{(l-1)-i} = \beta_{l-1} A^2_{l-1} \begin{pmatrix} \cos \theta_{l-1} \end{pmatrix} \), and \( S_{(l-1)-o} = \beta_{l-1} A^2_{l-1} \begin{pmatrix} \cos \theta_{l-1} \end{pmatrix} \). For the TE mode, \( \beta_0 = \sqrt{\varepsilon_{\omega} / |\mu_0|} \), \( \beta_1 = \sqrt{\varepsilon_{\omega} / |\mu_0|} \) for the TM mode, \( \beta_0 = \sqrt{\mu_0 / \varepsilon_{\omega}} \), \( \beta_1 = \sqrt{\mu_0 / \varepsilon_{\omega}} \), where \( \varepsilon_{\omega} \) is the dielectric constant of the
The frequency domain can be written as

\[ \mathcal{E}_{DBR}(t) = \mathcal{T}(t) + t_t r_t \mathcal{P} \left( t - \frac{2 z_{ol}}{c} \right) + t_t (r_t r_b) \mathcal{P} \left( t - \frac{2 L_{oc}}{c} \right) + \cdots, \]

where \( r_t \) and \( t_t \) are the reflection amplitude and transmission amplitude of the top DBR mirror, respectively. \( r_b \) is the reflection amplitude of the bottom DBR mirror with \( \text{monolayer MoS}_2 \) TFT, \( \mathcal{P}(t) \) is the electric amplitude against time for a single emission event (in either direction), \( z_{ol} \) is the distance between the OLED and bottom DBR mirror, \( L_{oc} = n_c L_{cav} \) is the optical length of the microcavity, \( n_c \) is the refractive index of the microcavity, and \( L_{cav} \) is the microcavity length. By using the Fourier transform, the emitted radiation from the top DBR mirror is transmitted and reflected by the two distributed Bragg reflectors (DBRs) of the microcavity. The field amplitude of the wave train emitted out from the top DBR mirror is given by [34,42]

\[ E_{DBR}(t) = \frac{t_t}{2\pi} \int_{-\infty}^{\infty} \mathcal{P}(t) \exp(\mathbf{i} \omega t) dt + \frac{t_t r_b}{2\pi} \int_{-\infty}^{\infty} \mathcal{P}(t - \frac{2 z_{ol}}{c}) \exp(\mathbf{i} \omega t) dt + \frac{t_t (r_t r_b)}{2\pi} \int_{-\infty}^{\infty} \mathcal{P}(t - \frac{2 L_{oc}}{c}) \exp(\mathbf{i} \omega t) dt + \cdots. \]

Neglecting the changes of the spontaneous time, the integral of eq. (7) through a change of variables, the forward emission intensity from the top side of the microcavity can be calculated by [34,42]

\[ |E_{DBR}(\lambda)|^2 = \frac{1 + R_b + 2 \sqrt{T_b/R_t} \cos \left( \frac{4 \pi n_r z_{ol}}{\lambda} \right)}{1 + R_b R_t - 2 \sqrt{T_b \bar{R}_t} \cos \left( \frac{4 \pi n_r L_{oc}}{\lambda} \right)} |T_t(\lambda)|^2, \]

where \( T_t = |t_t|^2 \) and \( R_t = |r_t|^2 \) are the transmittance and reflectance of the top DBR mirror, respectively, \( T_b = |t_b|^2 \) and \( R_b = |r_b|^2 \) are the transmittance and reflectance of the bottom DBR mirror with the MoS\(_2\) TFT, respectively. \( T_t \), \( R_b \), \( T_b \), and \( R_t \) are calculated by using the transfer-matrix method. By replacing the \( T_t, R_t, \) and \( R_b \) with \( T_b, R_b, T_t \), respectively, the forward emission intensity from bottom side of the microcavity can be obtained.

The light absorption and transmission of monolayer MoS\(_2\) in a flexible d-1DPC without OLED is investigated firstly. For comparison, we calculated the transmittance and absorbance of monolayer MoS\(_2\), as well as the absorbance of single-layer graphene (fig. 2(a)). The absorbance of monolayer MoS\(_2\) is about 6% to 30%, and its transmittance is about 70% to 90%. The absorbance of graphene is around 2.3%. The three-color principle was used in the general display technology. The same pixel was decomposed into three colored dots, red, green, and blue, through a filter or light resource with different colors. We investigated each of the three colors. The wavelengths of red, green, and blue light are 627, 516, and 470 nm, respectively [32–36]. All the color dots used different photonic crystal-structure parameters with \( M_u = M_d = 8 \).

The thicknesses of layers A, B, and C for the red photonic crystal are 89.4, 107.3, and 212.0 nm, respectively. The thicknesses of layers A, B, and C for the green photonic crystal are 73.9, 88.7, and 171.0 nm, respectively. The thicknesses of layers A, B, and C for the blue photonic crystal are 67.1, 80.5, and 158.0 nm, respectively. The corresponding transmittances of red, blue, and green light can also reach 99.5%, 99.4%, and 98.9%, respectively. The corresponding absorbance of monolayer MoS\(_2\) (graphene) in the microcavity are 0.35% (0.13%), 0.45% (0.10%), and 0.96% (0.13%), which are 20.2 times (17.7 times), 19.8 times (23 times), and 17.8 times (17.7 times) less than those in the non-microcavity monolayer MoS\(_2\) (graphene).

A strong localization effect of light occurred in the defective area of the photonic crystal (inset of fig. 2(d)). However, the light intensity is weakened in the special defective position because of the interference effect, thereby causing weak absorption. The microcavity resonance also
resulted in a transmittance close to 1. These characteristics can enhance the transmittance of monolayer MoS$_2$ film transistors, thereby improving the open ratio of display elements and reducing the effect of light absorption on the conductivity of monolayer MoS$_2$ and on/off ratio of film transistors.

Changing the number of cycles ($M_A$ and $M_B$) of A and B layers can regulate the absorption of monolayer MoS$_2$ (fig. 3). For example, in the green light, when the numbers of cycles in layers A and B increase simultaneously, the interference effect is more significant, but the absorption is lower. For $M_A = M_B = 7$, the absorptance of monolayer MoS$_2$ is about 0.58%; for $M_A = M_B = 10$, the absorptance of monolayer MoS$_2$ is only 0.28%, which is reduced by 31.8 times. In an asymmetric case ($M_A \neq M_B$), the absorptance and transmittance of monolayer MoS$_2$ are both reduced.

The resonance in the defective microcavity of the photonic crystal is sensitive to the thickness of the defective layer and incident angle (fig. 4). The resonance wavelength of the microcavity meets $M_0 \lambda_c = L_c \cos \theta'$; $L_c = n_c2d_c$ refers to the optical path length of the microcavity, $n_c$ and $d_c$ is the refractive index and thickness of the C layer; $M_0$ is a positive integer; and $\theta' = \arcsin \theta_i$ refers to the propagation angle in the defective layer, $\theta_i$ is the incident angle. Therefore, when the defective layer becomes thicker, the resonance wavelength will increase linearly. If $M_0$ is an odd number, the absorption of monolayer MoS$_2$ will be enhanced, and the maximum absorptance can reach 0.44. The corresponding resonance transmittance decreases. If $M_0$ is an even number, the absorption of monolayer MoS$_2$ will be inhibited, and the resonance transmittance can reach the maximum. When the incident angle becomes larger, the resonance wavelength shifts to a short-wave region. The resonance wavelength is determined by the propagation angle in the defective layer. Therefore, the sensitivity to the incident angle will depend on the index of refraction of the defective layer. If the index of refraction is higher, the resonance peak will change more slightly. The index of refraction of the defective layer is 1.5 (fig. 4). Thus, the defective layer is sensitive to the incident angle.

The microcavity-based TFT can be used in the traditional TFT display technology due to the fact that the thickness of the defective layer and the incident can be fixed. But for flexible OLED display technology, the thickness of the defective layer and the incident angle will be changed if the TFT is bent. This flexibility is unfavorable to the traditional display technology. However, microcavity-based OLED technology has been widely developing. Considering the localization effect of light, the quantum efficiency of OLED can be significantly improved by integrating OLED in the microcavity, thereby improving brightness and reducing power consumption [32–36]. If monolayer MoS$_2$ thin-film transistor is integrated with OLED in a microcavity, lights emitted by OLED will change synchronously with the change in the thickness of the microcavity and propagation angle of the light, thereby keeping high transmittance and low absorptance of monolayer MoS$_2$ unchanged (fig. 1(b)). Such integration is also favorable to reduce the monitor thickness. Given the simplified process and reduction of the pixel size, the integration can significantly improve the opening ratio of TFT, which cause low-power consumption.

Therefore, we investigated the emission intensity from the microcavity when the monolayer MoS$_2$ TFT is integrated with OLED in a microcavity. Numerical results are shown in fig. 5. To separate the emission source region, the TFT (monolayer MoS$_2$, one C layer, and graphene layer) and the bottom 1D photonic crystal DBR, as a whole, are treated as the bottom mirror. $L_{\text{abs}} = 344\, \text{nm}$ and the optical length of the microcavity is 516 nm. The distance

![Fig. 3](image_url) Effects of the number of cycles ($M_A$ and $M_B$) in A and B layers on (a) monolayer MoS$_2$ absorption and (b) d-1DPC transmission.

![Fig. 4](image_url) Influence of the thickness of the defective layer on (a) monolayer MoS$_2$ absorption and (b) d-1DPC transmission. Effect of incident angle on ((c), (e)) monolayer MoS$_2$ absorption and ((d), (f)) d-1DPC transmission.
from the emitting molecules to the bottom DBR mirror $z_{ol} = L_{cav}/2 = 172$ nm. The thickness of TFT and spacer layer is 171 nm. The imaginary part of the monolayer MoS$_2$ dielectric constant is either 0 (non-absorption, black solid line) or not 0 (absorption, colored lines). When monolayer MoS$_2$ ($d_m = 0$ nm) is located in the bottom side of the microcavity, the emission intensity is almost unchanged with or without absorption due to the ultralow absorption at 516 nm (inset of fig. 5(b)). When monolayer MoS$_2$ is 10 nm away from the bottom side of the microcavity ($d_m = 10$ nm), the emission intensity is almost unchanged. When monolayer MoS$_2$ is 88.5 nm away from the bottom side of the microcavity, the absorption becomes strong with significantly reduced emission intensity. The forward emission intensity from the top side of the microcavity is slightly larger than that from the bottom side of the microcavity due to the absorption of the bottom DBR mirror.

Finally, we discuss the influence of the $Q$-value of the microcavity and the achievement of the relative experiment.

The influence of the $Q$-value of the microcavity: The optical properties of a microcavity can be described by the $Q$-value. A larger $Q$-value means a stronger interference effect, which will lead to a higher peak value and a low valley value of the optical field distribution in the microcavity. Thus, a larger $Q$-value can reduce the absorption of the TFT and enhance the emission intensity from the OLED. Basing on the definition of the $Q$-value $Q = \omega_{0}/\Gamma$, we can conclude that greater $Q$-values mean smaller full width at half-maximum. Too smaller full width at half-maximum is adverse to the practical application.

Feasibility of the experiments: Organic flexible photonic crystals have been commercially produced before [32]. The growing and manufacturing technology for monolayer MoS$_2$ thin-film transistors also tends to be mature [5–9]; particularly, the method developed by Salvatore et al. can effectively transfer monolayer MoS$_2$ TFT to integrate with other microstructures [6]. Microcavity OLED-related manufacturing technologies, including microcavity integration, manufacturing, and connecting of electrodes, also continue to improve [32–36]; particularly, three-color OLED with organic flexible d-1DPC have been produced [32]. Hence, the development of microcavity-integrated monolayer MoS$_2$ film transistor and display technology of OLED is completely feasible.

In conclusion, the regulatory function of d-1DPC in the absorption and transmission of monolayer MoS$_2$ is investigat-  

This work was supported by the NSFC Grant Nos. 11364033 and 11264030, the NSF from the Jiangxi Province No. 2012BB212003, Science and Technology Project of Education Department of Jiangxi Province No. GJJ13005 and 2015chnu10, and the Invention Patent Foundation of Jiangxi Province under Grant No. 20143BBM26116.

References

[1] Janotti A. and de Walle C. G. V., Rep. Prog. Phys., 72 (2009) 126501.
[2] Sun Dong-Ming, Liu Chang, Ren Wen-Cai and Cheng Hui-Ming, Small, 9 (2013) 1188.
[3] Klaukas H., Chem. Soc. Rev., 39 (2010) 2643.
[4] Wang Q. H., Kalantar-Zadeh K., Kis A., Coleman J. N. and Strano M. S., Nat. Nanotechnol., 7 (2012) 699.
[5] Pu J., Yomogida Y., Liu K. K., Li L. J., Iwasa Y. and Takenobu T., Nano Lett., 12 (2012) 4013.
[6] Salvatore G. A., Münzenrieder N., Barraud C., Petti L., Zysset C., Bütte L., Ensslin K. and Tröster G., ACS Nano, 7 (2013) 8809.
[7] Pu J., Zhang Y., Wada Y., Wang J. T.-W., Li L.-J., Iwasa Y. and Takenobu T., Appl. Phys. Lett., 103 (2013) 023505.
