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High-efficient light absorption of monolayer graphene via cylindrical dielectric arrays and the sensing application

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ABSTRACT

The efficiency of graphene-based optoelectronic devices is typically limited by the poor absolute absorption of light. A hybrid structure of monolayer graphene with cylindrical titanium dioxide (TiO_2) array and aluminum oxide (Al_2O_3) spacer layer on aluminum (Al) substrate has been proposed to enhance the absorption for two-dimensional (2D) materials. By combining dielectric array with metal substrate, the structure achieves multiple absorption peaks with near unity absorbance at near-infrared wavelengths due to the resonant effect of dielectric array. Completed monolayer graphene is utilized in the design without any demand of manufacture process to form the periodic patterns. Further analysis indicates that the near-field enhancement induced by surface modes gives rise to the high absorption. This favorable field enhancement and tunability of absorption not only open up new approaches to accelerate the light-graphene interaction, but also show great potential for practical applications in high-performance optoelectronic devices, such as modulators and sensors.

1. Introduction

Over past few years, the graphene has attracted a great attention due to its remarkable electronic and optical properties i.e., the ultra-broad spectral response, ultra-thin atomic layer thickness and ultra-high carrier mobility [1–5], making it an ideal material for optoelectronic devices such as polarizers [6], modulators [7–14], capacitors [15], transistors [16], plasmonic components [17–22] and photodetectors [23]. However, for monolayer two-dimensional (2D) materials, there are typically two inherent defects that hinder the performance of optical devices. Firstly, the absolute absorption of monolayer is very small within the visible and near-infrared ranges, which limits the quantum efficiency and results in the low efficiency. Secondly, the monolayer graphene does not possess spectral selectivity because of the ultra-wide absorption spectrum ranging from the ultraviolet to terahertz [24–26].

Up to now, various technologies have been presented to improve the absorption of monolayer graphene. In the visible and near-infrared regions, the graphene is hard to support plasmonic resonance since the doping level is limited, so the absorption enhancement was normally realized by coupling it with resonant structures [27–35]. It has been reported that the plasmonic phenomenon in metal nanostructures have the potential to enhance the light absorption in graphene due to the near-field enhancement and high confinement of light [36–38]. Fang et al. observed an improvement in the photocurrent generation by introducing the metal antennas between graphene layers to excite plasmonic modes [36]. The deep metal grating was also utilized by Zhao et al. to enhance the graphene absorption [37] up to 70%. In addition, Zhu et al. found that the plasmonic coupling of a nanovoid array in the visible range could result in 30% enhancement of absolute light absorption and 700-fold enhancement of Raman response [38].

In this work, the cylindrical titanium dioxide (TiO_2) array sitting on aluminum (Al) substrate coated with graphene film were proposed and numerically investigated. Different from graphene-based structures reported before, the material of Al, which behaviors as a promising low-cost plasmonic material, is used as the substrate. Meanwhile, there is no demand to cut graphene into

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periodic patterns, which basically reduce the complexity in the process of manufacture. Furthermore, it was demonstrated that the absorption for 2D materials can be significantly enhanced by incorporating them into a PhC and an Al back reflector to completely block the transmission. Three absorption peaks can be observed at near-infrared wavelength, and the corresponding field properties were studied using the Finite Difference Time Domain (FDTD) method. In addition, the influence of structural parameters on the absorption was analyzed in detail.

2. Model and methods

The schematic diagram of cylindrical titanium dioxide (TiO_2) array sitting on aluminum (Al) substrate is shown in Fig. 1(a). Fig. 1(b) exhibits the cross-section view in *x*-*z* plane. A monolayer graphene is placed between an Al_2O_3 layer and a 2D TiO_2 periodic structure with hexagonal lattice. An Al layer is deposited at the back side of Al_2O_3 layer to block the transmission of incident light. The thickness of Al_2O_3 layer is denoted as *t*. The height and radius of cylindrical TiO_2 are *h* and *r*, respectively. *p* represents the period of TiO_2 array along *x* direction. The material properties of TiO_2 and Al_2O_3 are adopted from Palik's optical constants handbook [39]. The permittivity of Al is given by the Lorentz-Drude model [40]. The graphene layer is assumed as an infinitesimally thin surface with the surface conductivity σ_G calculated from Kubo formula [12,19,24]. It can be divided into intraband and interband contributions at finite temperature:

$$\sigma_G = \sigma_G^{intra} + \sigma_G^{inter}, \tag{1}$$

$$\sigma_G^{intra} = \frac{e^2}{4\hbar}\frac{i}{2\pi}\left\{\frac{16k_BT}{\hbar(\omega+i\Gamma)}\ln\left(2\cosh\left(\frac{\mu_c}{2k_BT}\right)\right)\right\}, \tag{2}$$

$$\sigma_G^{inter} = \frac{e^2}{4\hbar}\left\{\frac{1}{2}+\frac{1}{\pi}\arctan\frac{\hbar\omega-2\mu_c}{2k_BT} - \frac{i}{2\pi}\ln\frac{(\hbar\omega+2\mu_c)^2}{(\hbar\omega-2\mu_c)^2+(2k_BT)^2}\right\}. \tag{3}$$

In Eqs. (2) and (3), $\hbar = h/2\pi$ and k_B are the reduced Planck's constant and Boltzmann constant, respectively. *e* and μ_c are the electron charge and chemical potential, respectively. ω is the angular frequency. *T* denotes the temperature, and Γ stands for the momentum relaxation time due to the charge carrier scattering. The physical parameters of the graphene can be rationally set as $T = 300$ K, $\Gamma = 0.1$ meV, and $\mu_c = 0.15$ eV. The interaction between the light and graphene-TiO_2 is investigated by a 3D-FDTD method. The perfectly matched layer (PML) absorbing boundary conditions are utilized at the top and bottom of computational space, and the periodic boundary conditions are employed along *x* and *y* directions, respectively. The plane wave is defined as the light source and normally incidents to the array, and the electrical vector of plane wave is parallel to *x*-direction in simulation unless clarified. In the simulation, the thickness of monolayer graphene is assumed as 0.34 nm [41]. The absorbance $A(\omega)$ can be calculated by $A(\omega) = 1\text{-}R(\omega)\text{-}T(\omega)$, where $R(\omega)$ represents the reflectivity which is obtained from the numerical simulation. While $T(\omega)$ is the transmittance, and it reduces to be zero due to the block of reflective Al substrate.

3. Results and discussion

To develop photonics and metamaterials, one of the most inspiring aspects is to achieve desired optical properties by configuring structures beyond the intrinsic properties including materials. Al is employed as the back reflector to avoid incident light penetrating into metal film, which reduce the escaped power thus enhance the absorption to approach unity. A Fabry-Perot (FP) cavity can be formed between the back Al reflector and cylindrical TiO_2 array, giving rise to the interference and FP resonance. The structure therefore supports several guided resonant modes which can be coupled to external fields [42]. A guided resonant mode has its electromagnetic field strongly confined within the structure, and the field insides the structure can be significantly enhanced in the vicinity of the resonant frequency, indicating that the absorption of the structure can be greatly enhanced due to the field enhancement when the incident wave is coupled to a guided mode. The thickness of Al_2O_3 spacer layer is selected to achieve the spectral overlap of the two modes. The geometrical parameters are originally assumed as $h = 175$ nm, $t = 275$ nm, $r = 300$ nm and $p = 810$ nm, respectively.

Fig. 2 shows the absorption spectrum for structure under normal incidence. Three obvious absorption peaks can be observed, corresponding to the resonant wavelengths of 923 nm, 1112 nm, 1234 nm, which are marked as I, II and III respectively. Compared with the absorption spectrum for structure without graphene layer, it is found that the second absorption peak is mainly contributed due to the graphene. To reveal its underlying mechanism, the electric field patterns are necessary to quantitatively investigate. The electric field distribution relates to I mode is shown in Fig. 2(b). It is noted that the electric field is highly confined at the top of cylindrical TiO_2 due to the near-unity absorption in TiO_2 rather than

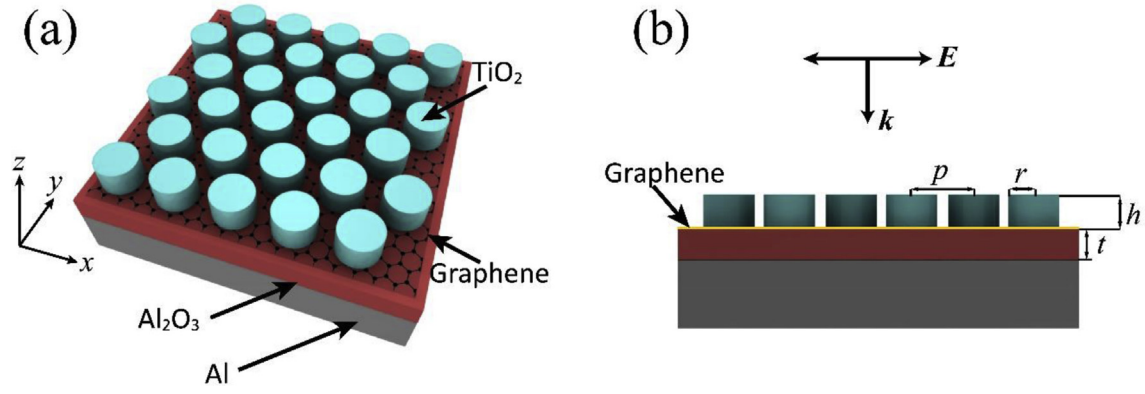

Fig. 1. (**a**) Schematic diagram and (**b**) cross-section view of cylindrical TiO_2 array packing on Al substrate coated with graphene film. The thickness of Al_2O_3 layer is denoted as *t*. The height and radius of cylindrical TiO_2 are *h* and *r*, respectively. The period of array along *x* direction is *p*.