SPECIAL TOPIC — Terahertz physics

High performance terahertz anisotropic absorption in graphene–black phosphorus heterostructure*

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(Received 14 May 2020; revised manuscript received 4 June 2020; accepted manuscript online 15 June 2020)

Graphene and black phosphorus have attracted tremendous attention in optics due to their support of localized plasmon resonance. In this paper, a structure consisted of graphene–black phosphorus heterostructure is proposed to realize terahertz anisotropic near-perfect absorption. We demonstrate that strong plasmonic resonances in graphene–black phosphorus heterostructure nanoribbons can both be provided along armchair and zigzag directions, and dominated by the distance between the graphene and black phosphorus ribbons. In particular, the maximum absorption of 99.6% at 10.2 THz along armchair direction can be reached. The proposed high performance anisotropic structure may have promising potential applications in photodetectors, biosensors, and terahertz imaging.

Keywords: graphene, black phosphorus, absorption, terahertz

PACS: 78.30.−j, 61.46.−w, 68.65.−k **DOI:** 10.1088/1674-1056/ab9cbf

1. Introduction

Since graphene was first exfoliated in 2004 by Novoselov *et al.*,[1] it has attracted considerable attention due to the unique properties and wide potential applications in nanoelectronics and nanophotonics.[2–6] Recently, studies show that propagating and localized surface plasmon modes can be excited in graphene-based nanostructures at terahertz range.[7,8] Graphene can be patterned into ring, circle, and cross-shaped arrays,[9–11] in which strongly enhanced light–graphene interactions have been demonstrated. Nevertheless, the absence of bandgap limits its more extensive applications in optical field.[12,13] As another new fashioned two-dimensional material, black phosphorus (BP) has not only high carrier mobility, but also bandgap and anisotropic properties, showing promising prospect in nanophotonics.[13–15] However, degradation under atmospheric conditions[16] and relatively weak interaction between monolayer BP and incident field are still challenges for applications in practice.[17–21] Recently, structures based on heterostructure of graphene and black phosphorus were reported to studied their electronic[22] and optical[23,24] characters. Nong *et al.* have demonstrated strong coherent coupling between graphene surface plasmons and anisotropic black phosphorus localized surface plasmons by a BP–spacer–graphene sandwich structure.[25]

In this paper, we propose a high performance anisotropic structure with graphene–black phosphorus (GB) heterostructure. According to the numerical simulation, strong and anisotropic absorption is realized at terahertz range. The maximum absorption reaches 99%. Furthermore, the absorption spectra can be tuned by Fermi energy and geometric parameters, such as the distance between the graphene and BP ribbons. These unique properties are not found in either alone monolayer BP or graphene.[26–29]

2. Structure and method

The schematic of monolayer BP atom structure is shown in Fig. 1(a), in which armchair direction is along x axis and zigzag direction is along y axis. Schematics of the periodic structures consisting of GB nanoribbons along armchair direction and zigzag direction are depicted in Figs. 1(b) and 1(c). The electric field of the incident light is along armchair direction (b) and zigzag direction (c), respectively. W is the width of the nanoribbons. P is the period of the periodic structure. The structural parameters are the same for the two structures. The two structures are made of perfect electrical conductor (PEC), dielectric layer, and GB nanoribbons. The cross sections of the structures are plotted in the insets. The dielectric substrate is placed on the metal mirror, and is covered by a layer of GB nanoribbons with period of P and width of W. Graphene is transferred onto BP using a three-axis micrometer stage and an optical microscope. Then the GB heterostructure is pattern into nanoribbons using UV lithography and oxygen plasma etching techniques.[30] The period and width are chosen to be $P = 210$ nm and $W = 150$ nm, respectively. In the CST (Computer Simulation Technology) software, both

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graphene and BP thicknesses are chosen to be 1 nm. The thickness of the dielectric is 2.1 μm and its refractive index is $n = 3.45$. PEC with 500 nm thick is used as a mirror to reflect light and prevent the transmission. So the absorptivity A is expressed by the formula $A = 1 - R$, in which R is the reflectivity. The dielectric layer between the GB heteostructure and the metal mirror forms a Fabry–Perot cavity to increase the interaction between light and the GB heterostructure.

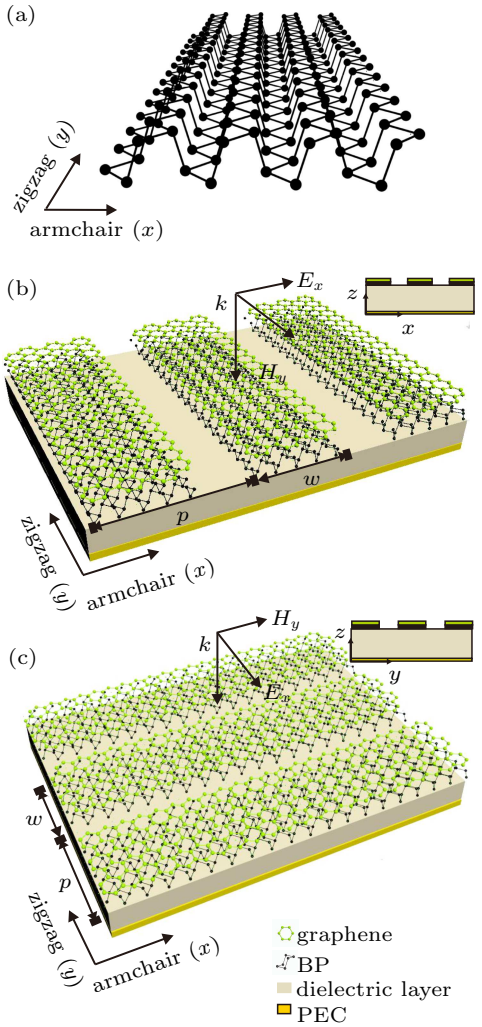

Fig. 1. Schematics of graphene–black phosphorus heterostructure. (a) Schematic of monolayer BP atom structure with armchair direction along x axis and zigzag direction along y axis. Schematic of the periodic structure consisting of GB nanoribbons along armchair direction (b) and zigzag direction (c).

According to the Kubo formula, the conductivity of graphene σ_{gra} can be expressed as $\sigma_{\text{gra}=}\sigma_{\text{intra}} + \sigma_{\text{inter}}$, which is contributed by interband and intraband transitions.[31,32] At the terahertz frequency $(h\omega \ll E_{\text{F}}), \sigma_{\text{inter}}$ is ignorable because it is much samller than σ_{intra} at room temperature. Then, the conductivity of graphene can be expressed as[33]

$$\sigma_{\text{gra}} = \frac{\mathrm{e}^2 E_{\text{F}}}{\pi\hbar^2} \frac{\mathrm{i}}{\omega + \mathrm{i}/\tau}. \tag{1}$$

The Fermi energy E_{F} is taken as 0.5 eV, and the relaxation time is choosen to be 1 ps. As shown in Fig. 1(a), BP has anisotropic electrical and optical properties because of its unique honeycomb atomic structure. According to the semiclassical Drude model, σ_j of monolayer BP can be described as[34]

$$\sigma_j = \frac{\mathrm{i}D_j}{\pi(\omega + \mathrm{i}\eta/\hbar)}, \tag{2}$$

where $\hbar$ is the Planck constant and η is the relaxation rate taken as 10 meV. D_j is the Drude weight given as $D_j = \pi e^2 n/m_j$ $(j = 1, 2)$, in which the electron doping $n = 1.9 \times 10^{13}$ cm^{-2}($E_{\text{F}} \approx 0.5$ eV), m_1 and m_2 are the electron masses along armchair direction and zigzag direction, respectively. For monolayer BP, $m_1 \approx 0.15m_0$ and $m_2 \approx 0.7m_0$ (m_0 is the static electron mass).[34]

3. Result and discussion

To study the different properties of alone graphene, BP, and GB heterostructure, the absorption spectra of the three materials are calculated as shown in Fig. 2. The absorption spectrum of monolayer graphene structure is plotted in Fig. 2(a), in which the resonance peak is located at 8.14 THz with the isotropic absorption of 56.94%. The optical response of graphene nanoribbons is isotropic because of the isotropic optical conductivity. The spectra of monolayer BP nanoribbons along armchair direction and zigzag direction are calculated, as shown in Fig. 2(b). The maximum absorptions of the BP nanoribbons along armchair direction and zigzag direction are 18.1% and 1.5%, respectively, indicating that the terahertz absorption of BP is anisotropic and relatively weak. In this paper, we try to combine the properties of graphene and BP by GB heterostructure. As shown in Fig. 2(c), the resonance peak is located at 11.2 THz with the absorption of 91.2% for the GB heterostructure nanoribbons along the armchair direction. For zigzag direction, the resonance peak is located at 9.3 THz with the absorption of 82.1%. Localized plasmon resonances can be excited at the nanoribbon structures along the two directions when the electric field of the incident light is perpendicular to the nanoribbons. The absorption relies on the localized plasmonic resonances of the GB nanoribbons.[24] The smaller electron mass along x direction than that along y direction indicates higher resonance frequency.[26] The results show a strong anisotropic resonance and a high absorption rate in the GB nanoribbons, which overcome the disadvantage of weak interaction between BP and the incident light.

The dependence of the absorption on the structure parameters is further investigated. Simulations of structures with different nanoribbons widths and periods are performed. With the period of 250 nm, we calculate the absorption of the structures with GB nanoribbons widths varying from 2 nm to 250 nm. The absorption spectra of the GB nanoribbons along armchair and zigzag directions are plotted in Figs. 3(a) and 3(b), respectively. The absorption peak positions show a redshift for the two directions when the width of the nanoribbons

increases. The phenomena indicate that the wide GB nanoribbons support the plasmon resonance at lower frequency. The absorption spectra with varying widths as a function of frequency are plotted in Figs. 3(c) and 3(d), respectively. The absorption peak intensity reaches the maximum of 98.1% with the width of 150 nm. These results show that the absorption intensity can be changed via regulating the width of the nanoribbons.

Additionally, simulations are performed for different periods ranging from $P = 150$ nm to 400 nm with fixed nanoribbons width of $W = 150$ nm. The absorption spectra of the GB nanoribbons in armchair and zigzag directions are plotted in Figs. 4(a) and 4(b), respectively. The absorption peak position shows a blue shift when the width of the nanoribbons along armchair direction increases. Moreover, as the gap (gap $= P - W$) between the nanoribbons becomes smaller, the resonance is strengthened and the absorption becomes larger. The absorption spectra for various periods of two directions are shown in Figs. 4(c) and 4(d). The absorption peak of periods from 210 nm to 290 nm reaches more than 90%.The above results show that the absorption peak intensity reaches the maximum value (99.6%) when $P = 230$ nm and $W = 150$ nm.

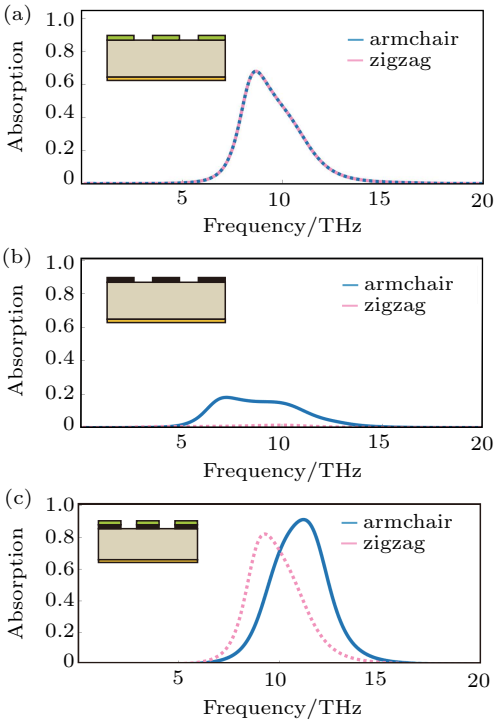

Fig. 2. Simulated spectra of absorption when graphene (a), monolayer BP (b), and GB (c) nanoribbons along armchair and zigzag directions. The insets are the schematic of the cross sections of these structures.

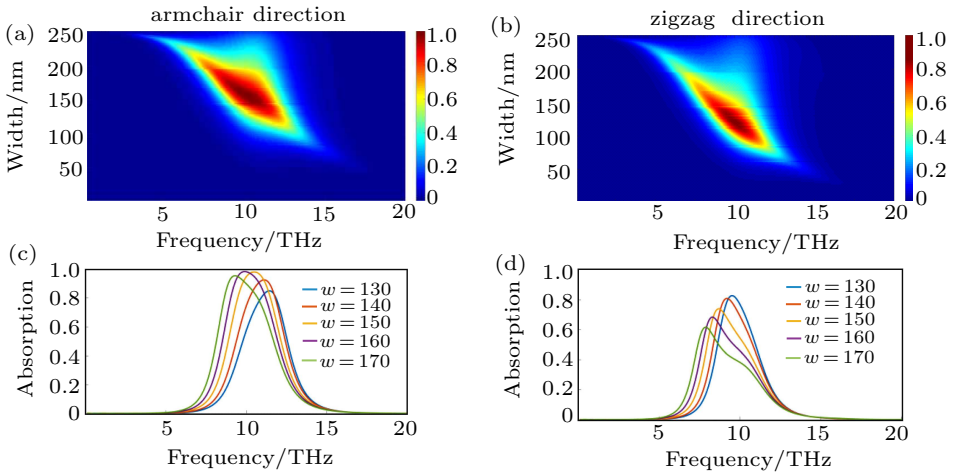

Fig. 3. Absorption map of GB nanoribbons along (a), (c) armchair direction and (b), (d) zigzag direction with various widths.

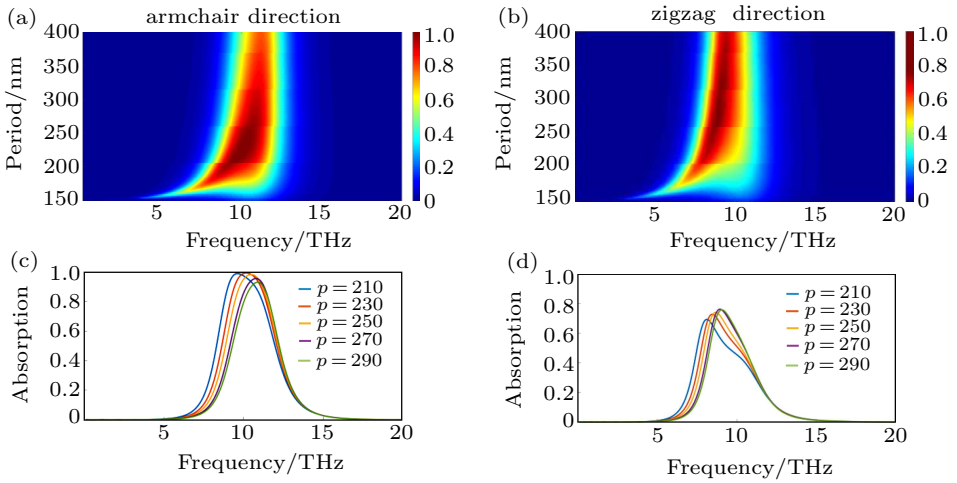

Fig. 4. Absorption map of GB nanoribbons along (a), (c) armchair direction and (b), (d) zigzag direction with various periods.

We then study the effect of the different Fermi energy of graphene in GB heterostructure on the absorption. With $P = 230$ nm and $W = 150$ nm, the Fermi energy of graphene is changed from 0.4 eV to 0.7 eV. The absorption spectra of nanoribbons along armchair and zigzag directions are shown in Figs. 5(a) and 5(b), respectively. For armchair direction, the absorption peak positions show a trend of blue-shift when the Fermi energy increases. Similarly for zigzag direction, the absorption peak positions show a blue-shift with Fermi energy increasing from 0.4 eV to 0.7 eV. The absorption spectra indicate that the strong anisotropic absorption of the structure exists with the increment of the Fermi energy.

By inserting a dielectric layer (its refractive index is the same as that of the dielectric layer in Fig. 1(b)) between graphene and BP nanoribbons, we study the influence of the distance between the two materials on the absorption spectra to understand the hybridization phenomenon. According to the above results, we choose nanoribbons parameters of perfect absorption as $P = 230$ nm , $W = 150$ nm, and $E_F = 0.5$ eV. The refractive index of the dielectric layer is 3.45. Parameter t is the thickness of the dielectric layer. The absorption spectra of the nanoribbons along two directions are shown in Fig. 6 when the thickness is changed from 0 to 20 nm. When the thickness of the dielectric layer is 0, the absorption peak of armchair and zigzag directions reaches maximum value 99.6% and minimum value 72.9%, respectively. With the increment of the thickness, the peak of armchair direction gets close to that of zigzag direction and almost overlaps each other at the thickness of 20 nm. In Fig. 6(a), positive and negative dipoles can be seen at the GB heterosturcture nanoribbons, indicating a strong localized plasmon resonance and THz absorption. For the edge surface plasmon modes, the electric field is mostly enhanced around the edges, which is similar to the edge modes in graphene ribbon structures.[35] At the same time, we note that the electric field profile of the vertical component E_z has a decreasing trend, consistent with the absorption of armchair direction. The results indicate that the anisotropism is strengthened in GB heterostructure (without dielectric layer between them).

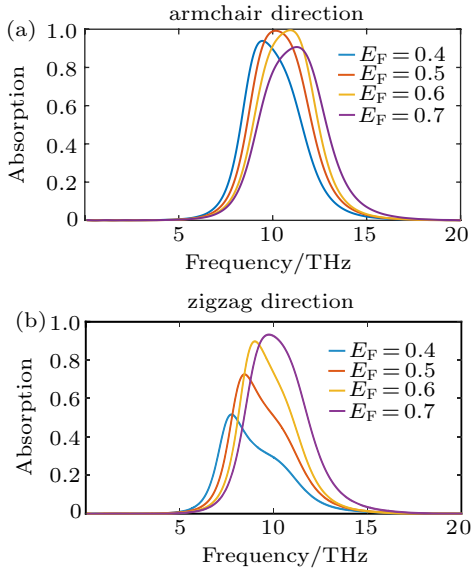

Fig. 5. Absorption spectra for various Fermi energy of graphene for GB nanoribbons along armchair direction (a) and zigzag direction (b).

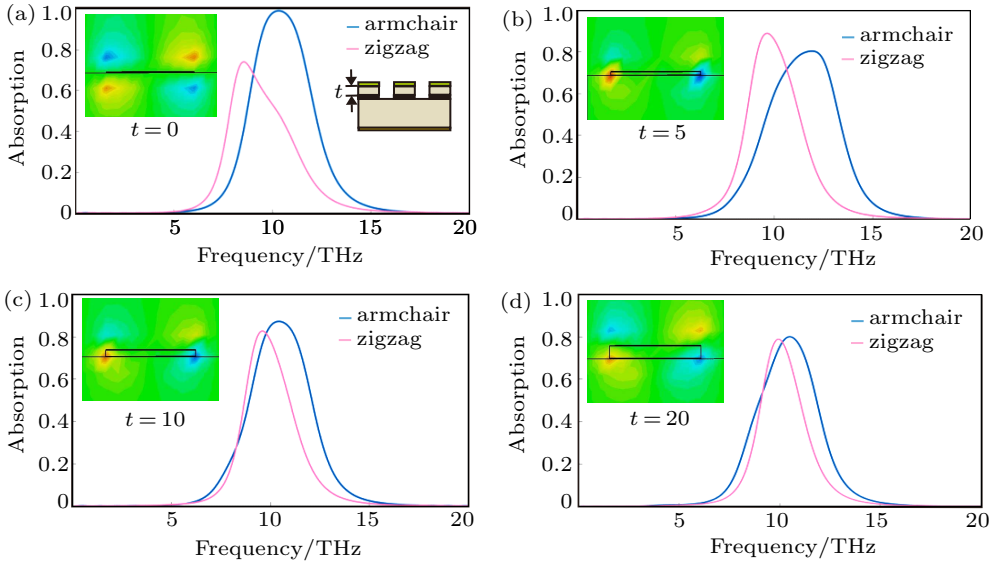

Fig. 6. Absorption spectra when nanoribbons along armchair and ziagzag directions. The distance between the graphene nanoribbons and the BP nanoribbons varies from $t = 0$ to 20 nm (a)–(d). Schematic of the cross section of the proposed structure is shown in the inset of (a). The insets are the side view electric field profile of the vertical component E_z at the resonance frequency for nanoribbons along armchair direction (the black rectangle is the inserting dielectric layer).

4. Conclusion

We theoretically propose a structure made of GB heteostructure. Different from monolayer BP or graphene, a strong anisotropic resonance and a high absorption rate can be achieved simultaneously in the GB nanoribbons along armchair and zigzag directions. The results suggest that by regu-

lating the width and period of the nanoribbons and the Fermi energy of graphene, the absorption peak intensity can reaches the maximum value (99.6%). Furthermore, we note that the anisotropism becomes strongest when the distance between graphene and BP nanoribbons is zero. This type of structure provides a new idea for high performance two-dimensional material plasmonic devices.

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