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Magnetic polaritons enhanced absorption of phosphorene in the near-infrared and visible region

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A B S T R A C T

We couple phosphorene with an Ag grating and exploit the resulting magnetic polaritons (MPs) to deliver the collected phonons to the phosphorene sheet. The power dissipation in the Ag grating and phosphorene is also investigated. The calculated results indicate that a large amount of power is absorbed by the phosphorene and results in about a 40-fold enhancement of absorption at λ = 595.5 nm. This design enables the increase of the absorption of phosphorene in the near-infrared (NIR) and visible region by varying the grating dimensions. In addition, the fundamental resonance frequencies excited by MPs in the Ag grating are explained by a LC circuit model.

1. Introduction

Two-dimensional atomic-layer systems, such as graphene, transition metal dichalcogenides (TMDCs) and so on, have attracted a significant attention due to their extraordinary functional properties and size–effect, which makes them as ideal materials not only for exploring novel physical phenomena but also for practical applications [1–5]. However, the lack of band-gap in graphene caused a high dark current in photodetectors when the bias voltage was injected to achieve high responsivity in the photoconductive mode [6,7]. Comparatively, most of the TMDCs exhibit relatively large direct bandgaps when in monolayer construction, rendering them unsuitable for near- or mid-infrared applications [8,9]. As for phosphorene, a single layer of black phosphorus (BP), with a band gap from 0.3 (bulk) to 2 eV (monolayer) [10,11], fills up the lacuna between zero-gap graphene and large-gap TMDCs, making it a promising material for near- and mid-infrared optoelectronics applications previously unharnessed by graphene and TMDCs. Moreover, BP has a host of novel electrical properties, including a higher carrier mobility (1000 $cm^2 V^{-1} s^{-1}$ at room temperature) compared to TMDCs monolayers, a high on-off ratio (10^5), strongly anisotropic electronic properties, as well as good current saturation in field-effect-devices [12,13]. These excellent properties make BP a great candidate for electronic, photonic, and thermoelectric devices. The broadband nonlinear optics response of few layer BPs and BP-based nonlinear optical devices had been recently reported by Fan's group [14,15]. Guo et al. have demonstrated BP mid-infrared detectors at 3.39 μm with high internal gain as well as an external responsivity of 82 A/W [16]. Recently, Youngblood et al. reported a photodetector based on multilayer BP, which showed a high responsivity and low dark current [17]. These experimental results show that such BP material is capable of sensing mid-infrared light due to its high photoresponse at mid-infrared wavelengths. However, a single layer BP only absorbs little light in the visible and near-infrared range region due to its atomically thin thickness. Besides, the absorption is further decreased by a factor $4/(1 + n)^2$ for films (this equation is valid for multi-layer structures) on a dielectric substrate of refractive index n [18]. Therefore, improving the absorption efficiency of mololayer BP (ML-BP) in the ultrafast photon detection is highly desirable and critical.

To efficiently enhance the absorption properties of two-dimensional materials, it is necessary to integrate them onto a planar photonic or into an optical microcavity device, by utilizing multiple passes of the trapped light through them [19–21]. Another method is taking advantages of plasmonic nanostructures to obtain a great enhancement in electromagnetic near-fields achieved by exciting surface plasmon polaritons (SPPs) on the metal-dielectric interface in response to incident radiation [22,23]. However, the enhancement is generally not very significant when the attenuated total reflection configuration is employed [24]. While the guided resonances in dielectric gratings can enhance two-dimensional materials absorption through critical coupling using photonic crystals [25,26], the enhancement achieved by this mechanism is usually narrowband and highly directionally sensitive.

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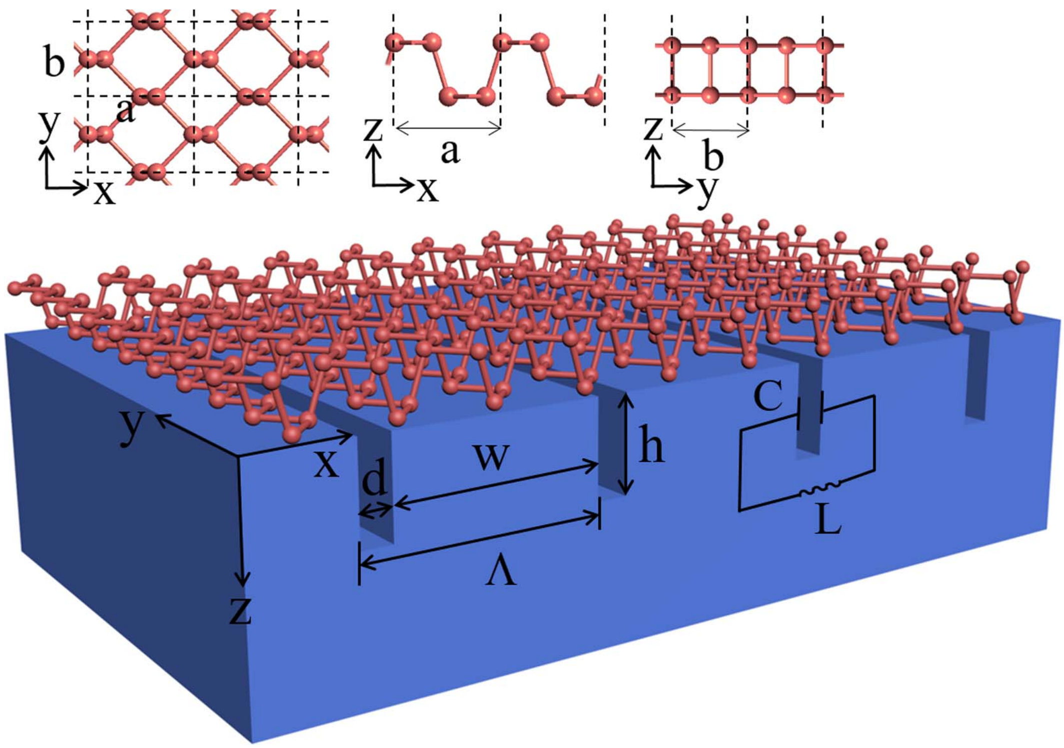

Fig. 1. Schematic diagram of the BP-covered Ag grating. The insets shows the top and side views of the atomic structure of ML-BP.

Along with the rapid advancement in metamaterials research, magnetic plasmon polaritons have been recognized as a mechanism for high-frequency magnetic response in some artificial nanostructures. The application of magnetic polaritons (MPs) has also been extended to cloaking materials [27], polarization switches [28], solar absorbers [29], negative refraction [30] and resonators [31]. In addition, MPs has also been employed to achieve extraordinary optical absorption in two-dimensional materials. Zhao et al. proposed utilizing MPs to enhance absorptance of graphene and showed that up to near 0.70 absorptance in graphene [32]. More recently, they achieved near-perfect absorption in hBN/metal grating hybrid anisotropic structures due to hBN strongly coupled with localized MPs [33].

In this letter, a method of enhancing the absorption of ML-BP is presented by using an Ag grating, which is due to the enhanced electromagnetic field when MPs are excited. Compared with other plasmonic nanostructures for graphene absorption enhancement [34] the proposed nanostructure provides extraordinarily large absorption efficiency for ML-BP. In addition, it has anticipated that metal-ion-modified BP might provide a new effective option for photonic applications toward high performances and enhanced stability [35]. It can be inferred that the ML-BP contacts to Ag grating could also enhance stability against oxidation and degradation.

2. Methods

In this work, the grating is illuminated by a normal incident plane wave polarized perpendicular to the grating (transverse magnetic, TM) since transverse electric (TE) cannot excite magnetic polaritons. The designed parameters for the structure include the grating period Λ, grating high h and trench d. For the 1D structure discussed here, the volume integration is carried out only in the x and z directions, and the structure is extended infinite in the z-direction for it to be opaque. Periodic and perfectly matched layer (PML) boundaries are applied in the lateral and vertical directions, respectively. Thus, the overall structure absorption is calculated by A = 1-R since the value of T (transmissivity) is zero, which is confirmed in the above part. The reflectance R is calculated by the Finite-Difference Time-Domain (FDTD) solutions.

The optical properties of Ag are obtained by using the Drude model $\varepsilon(\omega) = \varepsilon_\infty - \omega_p^2(\omega^2 + i\omega\gamma)^{-1}$ with the following parameters: high-frequency constant $\varepsilon_\infty = 3.4$, plasma frequency $\omega_p = 1.39 \times 10^{16}$ rad/s and scattering rate $\gamma = 2.7 \times 10^{13}$ rad/s. The electronic band-structures and accurate dielectric properties of ML-BP are calculated by using *ab initio* density function theory (DFT) combined with the GGA-PBE functional as implemented in the Atomistic-ToolKit (ATK) code [36]. We optimize ML-BP structure by LBFGS scheme until the maximum residual force is less than 0.01 eV Å^{-1} and stress tolerance is less than 0.001 eV Å^{-1}. The lattice parameters of a and b for the optimized ML-BP primitive cell are 4.41 Å and 3.32 Å, respectively, which are in good agreement with previous report [37]. The k-points of the cell, generated by the Monkhorst-Pack scheme [38], are set to 21 × 21 × 21, using a density mesh cut-off energy of 10 Ha. The electronic band-structures (not shown here) of the ML-BP show a direct band-gap of 0.83 eV, which is consistent with the other reports [11,39]. The Kubo-Greenwood formula is employed to calculate the susceptibility tensor [40]

$$\chi(\omega) = -\frac{e^2\hbar^4}{m^2\varepsilon_0 V\omega^2}\sum_{nm}\frac{f(E_m)-f(E_n)}{E_{mn}-\hbar\omega-i\hbar\Gamma}\pi_{nm}^i\pi_{nm}^j \quad (1)$$

The optical conductivity is related to the susceptibility tensor as $\delta(\omega) = -i\omega\varepsilon_0\chi(\omega)$, where ε_0 is the vacuum permittivity, e and m are the charge and effective mass of an electron, respectively, $\hbar$ is the reduced Planck constant, ω is the angular frequency, π_{nm}^i and π_{nm}^j are the *i*- and *j*-components of the dipole matrix element between state *n* and *m*, respectively, Γ is the broadening, and (…) is the Fermi function. The value of Γ is taken to be 0.1 eV. *V* is the volume related to the thickness of ML-BP. In the calculation, the thickness Δ of ML-BP is set as 0.52 nm. The equivalent dielectric constant of BP can subsequently be calculated via

$$\varepsilon(\omega) = 1 + i\sigma(\omega)/(\omega\varepsilon_0\Delta) \quad (2)$$