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Compact mid-infrared broadband absorber based on hBN/metal metasurface

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ABSTRACT

We propose a route to obtain broadband absorption in the mid-infrared region by coupling plasmon and phonon polaritons in compact hBN/metal metasurface. Here we show, with the assistance of the dispersion relation contours, that hybrid phonon-plasmon polaritons modes can exist in the hBN/metal heterostructures. By exciting these modes, i.e., hyperbolic phonon-plasmon polaritons in the Reststrahlen band and surface phonon-plasmon polaritons out of the Reststrahlen band of hBN, broadband near-perfect absorption can be achieved when carving the hBN/metal mutilayer into sawtooth gratings. The thickness of the gratings is about $\lambda_0/13$, which is an ultra-thin metasurface compared with previous works. The electric field and power dissipation density distributions are plotted to elucidate the mechanisms of the near-perfect absorption in different regimes. Furthermore, we present a detail analysis about the influence of changing the shape of gratings on the absorption performance and quantitatively evaluate the role hBN played in the absorber. The proposed route of designing broadband absorbers will benefit many practical applications, especially in the mid-infrared range.

1. Introduction

Broadband absorbers have been widely investigated for critical usages in many occasions, such as energy harvesting, detecting, radiative cooling, and so forth [1–6]. Broadband absorption can be realized by multi-resonances for both horizontally and vertically spaced resonance structures, which mainly consist of dielectric and metal materials [6–13]. Among them, sawtooth and pyramid structures have been widely researched as broadband absorbers [8–13]. In these structures, electromagnetic waves with long wavelengths are confined near the bottom of the sawtooth or pyramid, while those with short wavelengths are absorbed in the top part of the structures. This phenomenon has been explained as the slow wave modes in the effective hyperbolic metamaterials [11–13]. In general, it needs many metal-dielectric pairs to form hyperbolic metamaterials patterns, whose thicknesses are about $\lambda_0/6 \sim \lambda_0/5$ (λ_0 is the middle wavelength of the absorption band) [11,12].

Continuous efforts have been devoted to exploring new materials or structures, which can result in perfect broadband absorption by different mechanisms [14]. Recently, two-dimensional materials, such as hexagonal boron nitride (hBN), have been explored to design narrow band near-perfect absorbers [15–17]. It has been confirmed that hBN can support several higher order phonon-polaritonic waveguide modes inside the Reststrahlen band with hyperbolic dispersion, allowing extremely large k-values to exist [18,19]. In the context of 3D resonators, highly confined hyperbolic phonon polaritons (HPPs) in hBN nanocones and its anomalous internal reflections have also been reported recently [20,21]. For these reasons, strong resonance absorption can be achieved in one-dimensional gratings made of hBN due to HPPs [22]. However, the absorption band is usually quite narrow and sharply rolling in hBN absorbers [15,22], except with very sharp and adequate high (10 μm, about $1.5\lambda_0$) sawtooth structures [23], which may be difficult to fabricate. Moreover, light-matter interactions are deeply limited by the location of the Reststrahlen band which can provide hyperbolic dispersion, and only several discrete modes can be excited in regular condition.

In this work, we suggest a new route to design compact broadband absorbers in the mid-infrared region based on hBN/metal metasurface. In the proposed route, metal structures are introduced not only to excite and confine the HPPs in small hBN volumes, but also to combine surface plasmon polaritons (SPPs) and phonon-porlariton modes. Benefiting from such enhancement of light-matter interactions, the near-perfect absorption range can be greatly broadened when comparing with hBN/metal multilayer or uniform hBN gratings with the same structural parameters. It should be noted that the study of optical properties of hBN/metal heterostructures is also motivated by the following recent developments. First, the combination of plasmon and phonon-polaritons has promoted graphene/hBN heterostructure as

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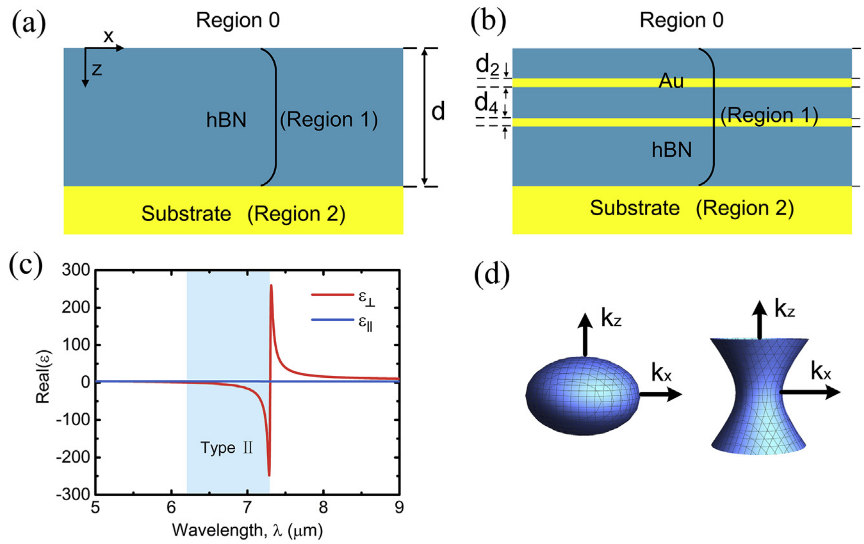

Fig. 1. (a) The uniform hBN structure with a thickness *d*. (b) Schematic of the prototypical hBN/metal heterostructure with bilayer metal plates embedded in an hBN slab. (c) Real part of the dielectric function of hBN. The shaded area indicates the hyperbolic region of hBN in the Reststrahlen band (6.21 μm < λ < 7.30 μm, hyperbolic type II). (d) Schematic illustration of the iso-frequency surface in the wave-vectors space of common ellipsoidal regime and hyperbolic type II regime.

interesting photonic systems to enhanced near-field thermal radiation [24,25], as well as tunable light-matter interactions [26,27]. Phonon modes of hBN can also be coupled to graphene plasmon, providing the possibility of observing near-perfect absorption at a specific frequency band and incidence angles [28]. Second, the hyperbolic phonon modes in hBN, which have been proposed for near-field optical imaging or focusing, can be excited by Au disk or the edge of the Au slab [18,29,30]. Although these studies provided the theoretical possibility to confine electromagnetic waves into small volumes, the work rendering hBN/metal heterostructure as broadband absorber has not been presented to the best of our knowledge.

2. Numerical modeling and theory

The prototypical model of uniform hBN structure and hBN/metal heterostructure studied in this work are shown in Fig. 1(a) and (b), respectively. In the hBN/metal heterostructure, bilayer metal plates, embedded in an hBN slab, are made of gold (Au) with thicknesses denoted as d_2 and d_4, and the hBN slab is separated into three layers with thicknesses d_1, d_3 and d_5. In both cases, the total thickness of the slab is *d*. The substrate is a Au film with a thickness that is sufficient to block all transmission. The theoretical model can be divided into three regions, consisting of region 0 (vacuum, <0), region 1 (hBN or hBN/metal, $0 < z < d$) and region 2 (Au, substrate, $z > d$), as shown in Fig. 1(a) and (b).

The real part of the dielectric function of hBN is shown in Fig. 1(c). The in-plane (denoted by ⊥) and out-of-plane (denoted by ||) dielectric functions are given by Ref. [26]:

$$\varepsilon_m = \varepsilon_{\infty,m}\left(1 + \frac{\omega_{\mathrm{LO},m}^2 - \omega_{\mathrm{TO},m}^2}{\omega_{\mathrm{TO},m}^2 - i\gamma_m\omega - \omega^2}\right), \tag{1}$$

where $m = \|, \perp$. The dielectric functions include the contributions from the in-plane phonon vibration ($\omega_{\mathrm{TO},\perp} = 1370\ \mathrm{cm}^{-1}$ and $\omega_{\mathrm{LO},\perp} = 1610\ \mathrm{cm}^{-1}$) and out-of-plane phonon vibration ($\omega_{\mathrm{TO},\|} = 780\ \mathrm{cm}^{-1}$ and $\omega_{\mathrm{LO},\|} = 830\ \mathrm{cm}^{-1}$). The other parameters used here are $\varepsilon_{\infty,\perp} = 4.87$, $\gamma_\perp = 5\ \mathrm{cm}^{-1}$, $\varepsilon_{\infty,\|} = 2.95$, and $\gamma_\| = 4\ \mathrm{cm}^{-1}$. The hyperbolic region means that the iso-frequency contour in the wavevector space is hyperboloid, as shown in Fig. 1(d), exhibiting many extraordinary properties, such as large energy density [31]. Out of the Reststrahlen band, the isofrequency surface is ellipsoid according to the dispersion relation [31]. In this work, we focus exclusively on the region around the Reststrahlen band (6.21 μm < λ < 7.30 μm, hyperbolic type II), where hBN can support HPPs. The permittivity of Au is taken from the handbook of optical constants of solids [32].

To visualize the underlying mechanism of broadband absorption, response functions and eigenmodes dispersions are conducted for both uniform hBN structure and hBN/metal heterostructures. In our theoretical model, we mainly consider the coupling condition between the surface plasmon polaritons and phonon polaritons. When the structure is composed with uniform hBN material in region 1, the complex reflection coefficient r_p of the structure is given by Ref. [33]:

$$r_p = \frac{r_{01} + r_{12}\exp(2ik_{z,1}d)}{1 + r_{01}r_{12}\exp(2ik_{z,1}d)}, \tag{2}$$

where subscript *p* signifies *p* polarization. Note that in the present study, the incident wave is assumed to be a plane wave whose magnetic field is in the *y*-direction, transverse magnetic (TM) waves. For transverse electric waves, the hBN behaves as an isotropic material only.

The reflection coefficient between media *a* and *b*, where $a = 0$ or 1 and $b = 0$, 1 or 2, can be obtained from Ref. [15]:

$$r_{ab,p} = \left(\frac{\varepsilon_{\perp,b}}{k_{z,b}} - \frac{\varepsilon_{\perp,a}}{k_{z,a}}\right) \Big/ \left(\frac{\varepsilon_{\perp,b}}{k_{z,b}} + \frac{\varepsilon_{\perp,a}}{k_{z,a}}\right), \tag{3}$$

where $k_{z,b} = (\varepsilon_{\perp,b}k_0^2 - \varepsilon_{\perp,b}\beta^2/\varepsilon_{\|,b})^{1/2}$ is the *z*-component of the wavevector in the given region. For regions with an isotropic material like regions 0 and 2, $\varepsilon_0 = \varepsilon_{\|,0} = \varepsilon_{\perp,0}$, $\varepsilon_2 = \varepsilon_{\|,2} = \varepsilon_{\perp,2}$. Here, β designates the magnitude of the wavevector in the *x*-*y* plane, k_0 and k_{z0} represent the magnitude and *z*-component of the wavevector in vacuum, respectively.

For hBN/metal heterostructures studied in this paper, there are 5 layers in region 1, consisting of three hBN layers and two Au layers. The complex reflection coefficient r_p of the structure can be solved by using the recursive method or transfer matrix method [33]. The imaginary part of the reflection coefficient $\mathrm{Im}(r_p)$, is introduced to elucidate the dispersion relation of a given structure [34]. The resonance location coincides with the peak of the function $\mathrm{Im}[r_p(\beta, \omega)]$, which allows the determination of the eigenmodes of the dispersion.

Rigorous coupled-wave analysis (RCWA) is a relatively straightforward method for obtaining the semi-analytical solution of Maxwell's equations, which has been widely used in calculating the radiative properties of periodic structures consisting of isotropic materials. Recently, the ordinary RCWA has been extended to an easy-to-implement anisotropic RCWA that allows the modeling of 2D periodic