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Manipulation of enhanced absorption with tilted hexagonal boron nitride slabs

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ABSTRACT

The wavevector of electromagnetic wave propagation in a hexagonal boron nitride (hBN) slab can be controlled by tilting its optical axis. This property can be used to manipulate the absorption in a hBN slab. By carefully analyzing the dependence of the absorptivity of a thin hBN slab on the tilted angle of its optical axis, we propose a structure that can realize great absorptivity enhancement in a band by stacking hBN slabs of different tilted angles. Our numerical results show that the absorptivity of a structure made of 91 stacked hBN slabs can be achieved higher than 0.94 in the wavenumber range from 1367 to 1580 cm^{-1} when the tilted angles of the slabs are properly arranged. The strong absorption is attributed to the combination of impedance matching at the slab interfaces and enlarged wavevectors in the slabs. This work reveals a novel way to realize strong absorption with anisotropic materials for applications in areas such as thermal radiative energy harvesting and conversion.

1. Introduction

As a two-dimensional Van der Waals crystal, hexagonal boron nitride (hBN) has attracted widespread attention due to its natural hyperbolicity and low-loss in mid-infrared [1–4]. It has been demonstrated theoretically and experimentally that a hBN slab of finite thickness can support multiple orders of hyperbolic phonon polaritons (HPPs) [5]. The excitation of HPPs has been employed to realize sub-diffraction imaging and focusing [6,7]. Recently, Zhao and Zhang [8–10] have revealed that the excitation of HPPs can also be used to create strong absorption. However, the larger wavevector of HPPs along the surface requires that grating structures should be employed for the excitation. Baranov et al. [11] proposed to realize perfect absorption in hBN slab by matching impedance between vacuum and the hBN slab. Wu et al. [12] theoretically demonstrated that the perfect absorption can be achieved and controlled by using a graphene-hBN crystal. Nevertheless, these latter two methods require the thickness of the structure to be infinite such that the transmission effect can be neglected. In this work, we propose an alternative method to greatly enhance the absorption in a thin hBN slab by tilting its optical axis. Nefedov et al. [13,14] have employed the same method to enhance the absorption of uniaxial metamaterials, which is related to matching of impedance at the surface and enlarged wavevector in the material. In their work, these two conditions were showed to be satisfied if one of the permittivity components is approximately 1 and the other is approximately – 1. However, it is not easy to design metamaterials to meet this strict requirement, not to mention natural materials. Besides, as they revealed, the incidence should be oblique in order to obtain perfect absorption. Different from Ref. [13], we investigate the absorption performance of a layered structure made of hBN slabs of different tilted angles when an electromagnetic wave is incident normally on it. We show that the absorptivity of the structure can be achieved higher than 0.94 in a band from 1367 to 1580 cm^{-1} with 91 stacked hBN slabs. By properly arranging the tilted angles of the stacked slabs, we show that matching of impedance at the slab interfaces can be, though not perfectly, satisfied. In addition, the wavevector in the slabs can be enlarged significantly around certain wavenumbers due to the tilted optical axis. These two factors contribute to the enhanced absorptivity in the structure, which is realized in a band when the tilted angle difference between adjacent slabs is small. Finally, the effect of slab thickness on the absorptivity of the structure is studied and we show that for the structure composed of 91 slabs, the large absorption can be obtained with each slab of only 20 nm thick.

2. Theory and computation

When the optical axis of hBN is along the z-axis of the coordinate system xyz, its permittivity tensor can be expressed as [15]

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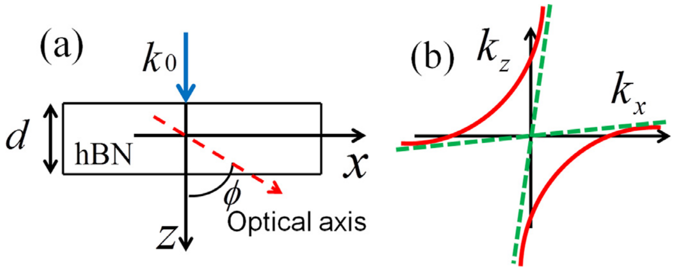

Fig. 1. (a) Schematic of the coordinates, the optical axis of hBN is tilted off the z-axis by an angle ϕ in the x-z plane. (b) The asymmetric isofrequency curves for the tilted hBN.

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_\perp & 0 & 0 \\ 0 & \varepsilon_\perp & 0 \\ 0 & 0 & \varepsilon_{||} \end{pmatrix}, \quad \varepsilon_m = \varepsilon_{\infty,m}\left(1+\frac{\omega_{LO,m}^2-\omega_{TO,m}^2}{\omega_{TO,m}^2-\omega^2+j\omega\Gamma_m}\right), \tag{1}$$

where $m=\perp,||$ indicates the component perpendicular or parallel to the optical axis. ω is wavenumber, the other parameters are $\omega_{TO,\perp}=1370$ cm^{-1}, $\omega_{TO,||}=780$ cm^{-1}, $\omega_{LO,\perp}=1610$ cm^{-1}, $\omega_{LO,||}=830$ cm^{-1}, $\varepsilon_{\infty,\perp}=4.87$, $\varepsilon_{\infty,||}=2.95$, $\Gamma_\perp=5$ cm^{-1} and $\Gamma_{||}=4$ cm^{-1}. When the optical axis is tilted off the z-axis by an angle ϕ in the x-z plane, as shown in Fig. 1(a), the permittivity tensor of hBN can be written as [16]

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & 0 & \varepsilon_{xz} \\ 0 & \varepsilon_{yy} & 0 \\ \varepsilon_{zx} & 0 & \varepsilon_{zz} \end{pmatrix} = \begin{pmatrix} \varepsilon_\perp\cos^2\phi+\varepsilon_{||}\sin^2\phi & 0 & \left(\varepsilon_{||}-\varepsilon_\perp\right)\sin\phi\cos\phi \\ 0 & \varepsilon_\perp & 0 \\ \left(\varepsilon_{||}-\varepsilon_\perp\right)\sin\phi\cos\phi & 0 & \varepsilon_{||}\cos^2\phi+\varepsilon_\perp\sin^2\phi \end{pmatrix}. \tag{2}$$

Here we consider the incidence wave is a TM wave with the x-z plane as the plane of incidence. In this case, there is no polarization coupling in the slab and for a transverse electric (TE) wave, the slab behaves like an isotropic medium with a permittivity of $\varepsilon_\perp$, regardless of the tilting [16]. In general, when the incidence angle is θ, the parallel wavevector component is $k_x=k_0\sin\theta$, where $k_0=\omega/c$ and c is the speed of light in vacuum. The relation between the parallel and vertical components of the wavevector in the tilted hBN is [16]

$$\varepsilon_{zz}{k_z}^2+2\varepsilon_{xz}k_xk_z+\varepsilon_{xx}{k_x}^2=\varepsilon_{||}\varepsilon_\perp{k_0}^2. \tag{3}$$

The diagram in Fig. 1(b) illustrates the isofrequency curves governed by Eq. (3), when $\varepsilon_{||}$ and $\varepsilon_\perp$ have opposite signs. We can see that the isofrequency curves are asymmetric about the two wavevector components k_x and k_z. When the tilted angle is zero, then $\varepsilon_{xz}=0$, Eq. (3) reduces to

$$\varepsilon_{||}{k_z}^2+\varepsilon_\perp{k_x}^2=\varepsilon_{||}\varepsilon_\perp{k_0}^2. \tag{4}$$

This relation has been studied in many papers [7,10,17]. One conclusion about this relation is that if a large wavevector is to be achieved, the vertical and the parallel wavevector components must be large simultaneously. In contrast, if we consider the parallel wavevector component $k_x=0$ in Eq. (3), we obtain

$$k_z=k=\sqrt{\frac{\varepsilon_{||}\varepsilon_\perp}{\varepsilon_{||}\cos^2\phi+\varepsilon_\perp\sin^2\phi}}k_0. \tag{5}$$

The above equation indicates that the wavevector can be large enough if $\varepsilon_{zz}=\varepsilon_{||}\cos^2\phi+\varepsilon_\perp\sin^2\phi$ is very small. This is possible when $\varepsilon_{||}$ and $\varepsilon_\perp$ have opposite signs and the value of ϕ is properly selected. The large wavevector in this case is illustrated schematically in Fig. 1(b).

For conciseness, we defined under normal incidence an apparent permittivity ε_a as

$$\varepsilon_a=\frac{\varepsilon_{||}\varepsilon_\perp}{\varepsilon_{||}\cos^2\phi+\varepsilon_\perp\sin^2\phi}, \tag{6}$$

such that $k_z=\sqrt{\varepsilon_a}k_0$ in the slab. In this paper we investigate the behavior of the tilted hBN in the wavenumber range from 1350 to 1600 cm^{-1}. hBN exhibits the property of hyperbolicity in the band from 1370 to 1600 cm^{-1}. The ε_a varying with wavenumber and the tilted angle is shown in Fig. 2. It can be seen that when the tilted angle is zero, the imaginary part of the permittivity is rather small in the hyperbolic band except for wavenumbers close to $\omega_{TO,\perp}$. When the tilted angle is not zero, the wavenumber for maximum value of $\mathrm{Im}(\varepsilon_a)$ changes with the tilted angle, and it moves towards higher wavenumber when the tilted angle increases. According to Eq. (6), a large amplitude of ε_a will ensure that the wavevector is also large in the slab. The property of the enhanced wavevector shifting with the tilted angle makes it potential to achieve strong absorption in hBN at tunable wavenumbers.

We study the absorption property of layered structures made of hBN slabs with varied tilted angles of the optical axis for normal incidence of a TM plane wave on the surface of the structure. For this purpose we adopt the transfer matrix method [18,19] for calculating the reflectivity and transmissivity of the structure. Then the absorptivity of the structure can be obtained by subtracting the reflectivity and the transmissivity from one, according to Kirchhoff's law [20].

3. Results and discussion

We first calculate the absorptivity of a hBN slab of thickness 20 nm as a function of wavenumber and the tilted angle for normal incidence of a TM plane wave from air. The result is shown in Fig. 3(a). The bright color in the graph indicates large absorption, which is in accordance with the behavior of ε_a depicted in Fig. 2. Because the reflection at the interface between air and the hBN slab is large due to the impedance mismatching, the maximum absorptivity does not exceed 0.5. We also investigate the impact of the slab thickness on the absorption. Taking wavenumber 1527 cm^{-1} as an example, this point corresponds to the maximum amplitude of ε_a when the tilted angle is 45°. Fig. 3(b) shows the absorptivity as a function of the slab thickness. It can be seen that an absorptivity peak of 0.5 appears at 20 nm. This is due to the combination of the enlarged wavevector and the Fabry–Perot (FP) resonance in the slab. The FP quantization condition can be written as [15]

$$\beta_a+\mathrm{Re}(k_z)d=m\pi, \tag{7}$$

where m is an integer, d is the thickness of the hBN slab, $\mathrm{Re}(k_z)$ is the real part of k_z. β_a represents the phase of the reflection coefficient r_a at the air/hBN interface, which is expressed for normal incidence as

$$r_a=\left(\sqrt{\varepsilon_a}-1\right)/\left(\sqrt{\varepsilon_a}+1\right). \tag{8}$$

The slab thickness of 20 nm satisfies the FP resonance condition with $m=1$. As the slab thickness increases further, the absorptivity curve does not show higher-ordered FP resonances, but saturates at a value around 0.21. This is because the imaginary part of k_z is so large that the wave decays very fast during propagation in the slab. In fact, when the slab is as thick as 441 nm, it also satisfies the FP resonance condition. But the backward propagating wave in the slab by reflection at the second interface is too weak to produce strong interference with the forward propagating wave. Therefore, the absorption peaks are flattened and, as a consequence, the maximum absorptivity corresponds to the first-ordered FP resonance.