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RAPID COMMUNICATION

Extinction mechanisms of hyperbolic h-BN nanodisk*

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We applied the finite element method to calculate the extinction spectrum of single hyperbolic hexagonal boron nitride (h-BN) nanodisk. We show that the hyperbolic h-BN nanodisk exhibits two extinction mechanisms in the mid-infrared region. The volume confined phonon polaritons resonances of the nanodisk give rise to a series of weak extinction peaks. The localized surface phonon polaritons lead to a robust dipolar extinction, and the extinction peak position is tunable by varying the size of the h-BN nanodisk. These findings reveal the mechanisms of the interaction between light and resonant h-BN nanodisk, which are essential for h-BN related opto-electromagnetic applications.

Keywords: extinction spectra, hexagonal boron nitride (h-BN), phonon polaritons, finite element method

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1. Introduction

The interaction of light with noble metal leads to resonant enhancement of the local electromagnetic field when the size scale of the metal structure is close to the wavelength of the incident light.[1–3] Surface plasmons are the collective excitations of the coupling between photon and electron,[4–6] and one can utilize the localized surface plasmons resonance in a metallic nanostructure to enhance the light–matter interaction.[7–12] The strong light–mater interaction on the resonant metallic structure has attracted lots of attention for sensing and spectroscopic applications[13–19] in recent years. However, in the infrared region, the noble metals perform as a nearly perfect conductor and reflect most of the incident light.[20] Similar to the surface plasmons in metal, the surface phonon polaritons localize at the boundary of the polar material and give rise to antenna effects in the infrared region.[8,20–22] More importantly, the relaxation time of the phonon quasiparticle is about one order longer than that of the electron counterpart, which is critical for optical and electronic applications.[8,21,22] Hexagonal boron nitride (h-BN) is a 2-dimensional van der Waals material with a hyperbolic dispersion permittivity, supporting two types of phonon polaritons in the corresponding Reststrahlen band,[6,23,24] and the excellent thermal[25] and chemical stabilities[26,27] of h-BN enable to fabricate guaranteed nanophotonic devices. Recently, the hyperbolic phonon polaritons of h-BN nanocone[28] and h-BN linear waveguide[29] demonstrated functionality in potential infrared nanophotonic applications. Furthermore, the metasurface consisted of the array of h-BN strips has been studied for controlling light in nanophotonic applications.[30] Therefore, researching and understanding the electromagnetic properties of a single h-BN nanostructure offer a guideline to design various h-BN polaritons related applications.

In this work, we studied the extinction features of a single h-BN nanodisk with 20 nm diameter and 2 nm thickness via the finite element method. The parameters of the h-BN disk assure that both the extinction effects of volume and the surface phonon polaritons are sharp and distinct upon excitation.[31] At the same time, the demand for calculation remains minimum. From the numerical simulation, we detected two origins accounting for the extinction property of the h-BN nanodisk, the volume confined phonon polaritons and the localized surface phonon polaritons (LSPhP), respectively. The volume confined phonon polaritons are excited from the disk edge and exhibit Fabry–Perot resonances that lead to a series of resonant peaks corresponding to different resonance orders. However, the localized surface phonon polaritons result in a distinct dipolar sharp resonant peak that can be precisely modulated by varying the structure parameters in the mid-infrared region. The quality factor of the LSPhP resonant extinction peak is about 193, and the electromagnetic field enhancement is about 40. The position of the dipolar resonance peak is related to the level of dipole polarization of the metallic h-BN disk. The tunable extinction peak, the high-quality factor of the extinction peak, and the strong electromagnetic field enhancement factor make the h-BN nanodisk a promising candidate for applications in the mid-infrared antenna, molecular sensing, and enhanced spectroscopy. The different extinction mechanisms

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and excitation conditions offer versatile ways to manipulate light at the nanoscale.

2. Method

The extinction spectrum of the h-BN nanodisk was calculated by the finite element method implanted in the Comsol multiphysics software. In the numerical simulation model, the nanodisk was immersed in a background medium (vacuum in our simulation model), and a linear polarized plane wave was illustrating on the nanodisk. The scattering and absorption cross-sections σ_{sc} and σ_{abs} are calculated[32,33] by

$$\sigma_{sc} = \frac{1}{I_0}\iint \boldsymbol{n}\cdot\boldsymbol{P}\mathrm{d}S, \tag{1}$$

$$\sigma_{abs} = \frac{1}{I_0}\iiint Q\mathrm{d}V, \tag{2}$$

where $\boldsymbol{n}$ is the normal vector pointing outwards from the h-BN disk, $\boldsymbol{P}$ is the Poynting vector, and I_0 is the intensity of the incident light. The integral in Eq. (1) is taken over the surface of the disk. Q is the power loss density in the disk, and the integral is taken over its volume. Thus, the extinction cross-section is the sum of these two terms

$$\sigma_{ext} = \sigma_{sc} + \sigma_{abs}. \tag{3}$$

The electromagnetic response of a material to light is related to its permittivity. h-BN is a 2-dimensional layered van der Waals material, and the permittivities of h-BN parallel and perpendicular to the layer are anisotropic. The permittivity of h-BN can be written as a Lorentz model:[6,24]

$$\varepsilon_i(\omega) = \varepsilon_{i,\infty}\left(1 + \frac{\omega_{i,\mathrm{LO}}^2 - \omega_{i,\mathrm{TO}}^2}{\omega_{i,\mathrm{TO}}^2 - \omega^2 - \mathrm{i}\omega\gamma_i}\right), \tag{4}$$

where $i = \mathrm{t}, z$ represent the in-plane and out-of-plane layers, $\varepsilon_{i,\infty}$ is the high-frequency dielectric permittivity, γ_i is the phonon damping constant in crystal, and $\omega_{i,\mathrm{LO}}$ ($\omega_{i,\mathrm{TO}}$) is the frequency of the longitudinal (transverse) optical phonon.

3. Results and discussion

Figure 1 presents the real parts of the in-plane permittivity $\mathrm{Re}(\varepsilon_t)$ and out-of-plane permittivity $\mathrm{Re}(\varepsilon_z)$ of h-BN. It shows that in the upper (lower) Reststrahlen band, the in-plane permittivity $\mathrm{Re}(\varepsilon_t)$ is negative (positive) and the out-of-plane permittivity $\mathrm{Re}(\varepsilon_z)$ is positive (negative). As h-BN is a layered material, we firstly investigate the property of the upper Reststrahlen band, which has a broader band region supporting the phonon polaritons than the lower Reststrahlen band.

For an out-of-plane polarized incident light, the extinction cross-section of the h-BN nanodisk with 20 nm diameter (D) and 2 nm thickness (h) is shown in Fig. 2(a). The distinct feature is a series of resonant peaks appearing in the extinction spectrum. In Figs. 2(b)–2(d), the side views of the near-field distribution of electric field $|E|$ at corresponding resonant frequencies are plotted, where the volume confined phonon polaritons get excited at the edge of the nanodisk[34] and oscillate in the h-BN disk. The propagation angle[6,28] θ (to the optical axis) of the polaritons rays (the red arrows shown in Figs. 2(b)–2(d)) depends on the frequency ω, where $\tan\theta(\omega) = \mathrm{i}\sqrt{\varepsilon_t}/\sqrt{\varepsilon_z}$. Therefore, different polaritons lead to Fabry–Perot resonance when the propagation angle is equal to specific values, i.e., $|\tan\theta(\omega)| = D/2mh$ ($m = 1, 2, 3, \ldots$). At different resonant order m, the volume confined phonon polaritons rays propagate inside the h-BN nanodisk and result in a Fabry–Perot resonance pattern. The side views of the near-field distribution of magnetic field $|H|$ at the corresponding resonant frequencies shown in Figs. 2(e)–2(g) reveal the

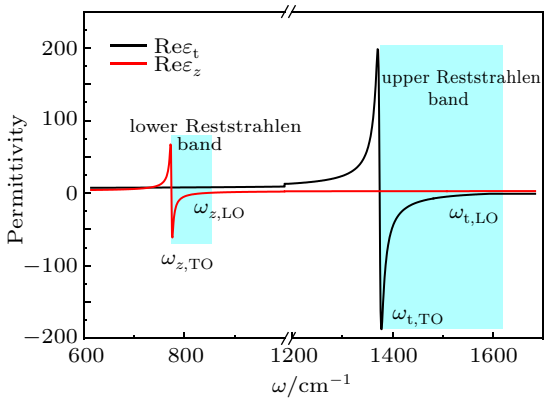


Fig. 1. The real parts of the in-plane permittivity $\mathrm{Re}(\varepsilon_t)$ and out-of-plane permittivity $\mathrm{Re}(\varepsilon_z)$ of h-BN.

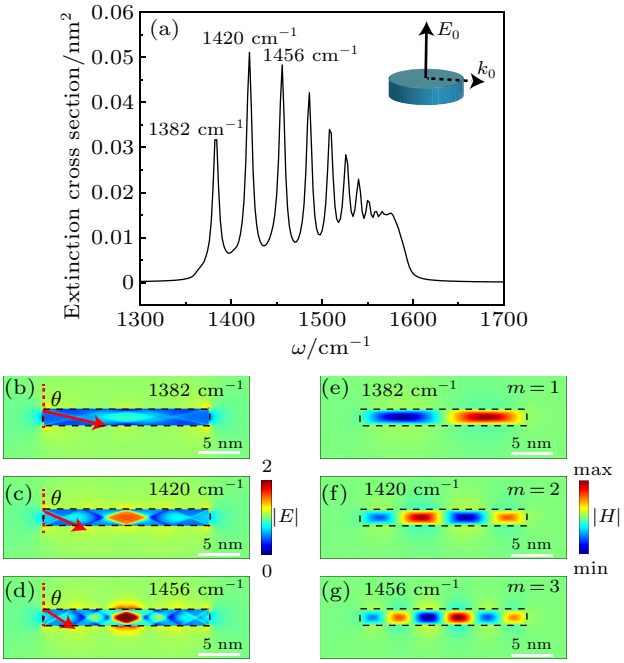


Fig. 2. Electromagnetic response of h-BN nanodisk to out-of-plane polarized incident light. (a) Extinction spectrum of h-BN disk with 20 nm diameter and 2 nm thickness under an out-plane polarized incident plane wave. Inset: The schematic of incident light illuminating on the h-BN nanodisk. (b)–(d) Side views of the near field distribution of electric field $|E|$ at different frequencies. (e)–(g) Side views of the near field distribution of magnetic field $|H|$ at different frequencies corresponding to (b)–(d). The black dashed line indicates the boundary of the nanodisk. The scale bar is 5 nm.

distinct Fabry–Perot resonant patterns of the magnetic field with different resonant order m. The extinction spectrum is similar to the nano-FTIR spectrum of a h-BN nanocone, which also shows a series of resonant modes in the nanocone.[28,35] Therefore, this Fabry–Perot resonance extinction offers an alternative perspective to understand the nano-FTIR spectra of the h-BN nanostructure.

When the incident light is in-plane polarized, only a sharp extinction peak appears at the frequency of 1444 cm^{-1}. The full width at half maximum (FWHM) of the peak is 7.48 cm^{-1}, which leads to a high-quality factor $Q = \omega/\Delta\omega = 193$, higher than that of most metals[36] and semiconductors.[22] The top view and side view of the near-field distribution of the normalized electric field $|E/E_0|$ are shown in Figs. 3(b) and 3(c), respectively. The distinct dipolar distribution of the electric field shown in the top view and side view figures indicates a dipolar resonance mode at the frequency of 1444 cm^{-1}. The electric field intensity in the near-field shows an enhancement factor ($f = |E/E_0|$) as high as 40 at 2 nm outside the disk. The polaritons rays inside the h-BN disk in Fig. 3(c) show that the volume confined phonon polaritons propagate inside the disk, whose contribution is negligibly in the extinction spectrum in Fig. 3(a). Compared to Fig. 2(a), the extinction cross-section originated from this dipolar resonance extinction is three orders of magnitude more robust than the volume confined phonon polaritons extinction. Therefore, the extinction spectrum is dominated by the dipolar extinction.

Surface phonon polaritons are the quasiparticles from the coupling between the photon and the optical phonon of the polar crystal, which belong to surface excitations. The oscillating surface phonon polaritons exhibit a large localized electric field confined at the interface of the polar crystal. The dipolar electric field distribution is localized at the boundary of the h-BN disk, which is similar to that of the localized surface phonon polaritons in a single SiC disk.[8] The surface-confined phonon polaritons in the upper Reststrahlen band of linear h-BN antenna[29] and ribbon[37] can manifest stronger field confinement than the volume phonon polaritons modes. From the dipolar mode pattern[8] and near-field distribution of the h-BN disk in Figs. 3(b) and 3(c), we attribute this dipolar extinction to the consequence of the localized surface phonon polaritons resonance similar to previously reported results[8,22] in the phonon crystal. For the localized surface phonon polaritons resonance in a metallic nanoparticle, the dipole polarizability is[9,33]

$$\alpha(\omega) \sim 3\varepsilon_{\rm m}(\omega) V_{\rm NP} \frac{\varepsilon(\omega) - \varepsilon_{\rm m}(\omega)}{\varepsilon(\omega) + \chi\varepsilon_{\rm m}(\omega)}, \tag{5}$$

where ω is the frequency of the incident light, $\varepsilon_{\rm m} = 1$ is the permittivity of the surrounding medium (air in our work), $V_{\rm NP}$ is the volume of the nanoparticle, χ is a geometrical factor, and $\varepsilon(\omega)$ is the complex in-plane permittivity of h-BN. The polarizability reaches the maximum when $\varepsilon(\omega) = -\chi\varepsilon_{\rm m}(\omega)$, which is called the Frohlich condition, this induces a resonance extinction peak in the spectra. The geometrical factor χ is related to the shape of the particle, and $\chi = 2$ for a sphere and $\chi = D/h$ for a disk.[38]

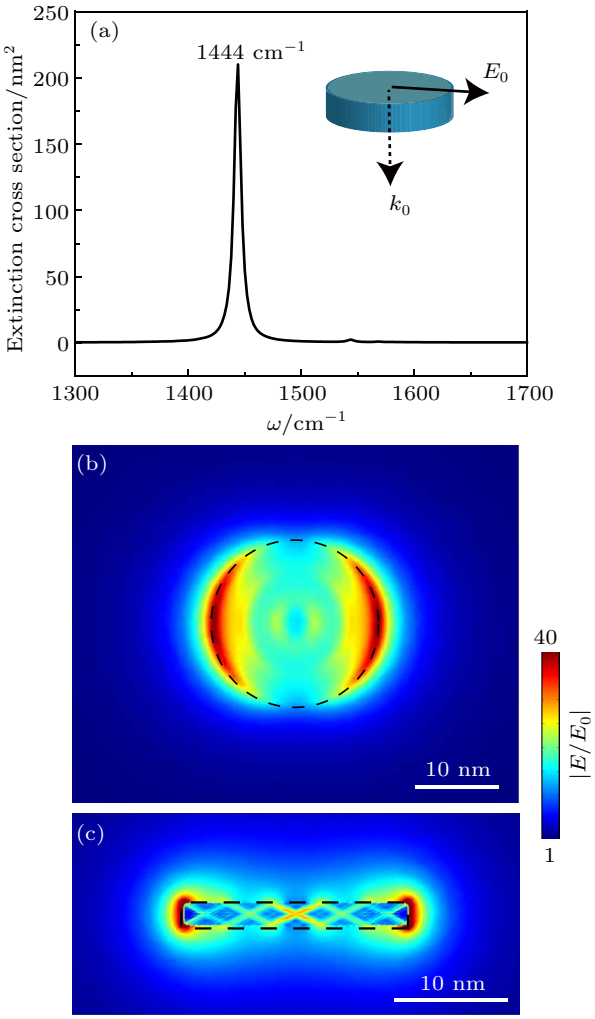


Fig. 3. Electromagnetic response of h-BN nanodisk to in-plane polarized incident light. (a) Extinction spectrum of a h-BN disk with 20 nm diameter and 2 nm thickness under an in-plane polarized incident plane wave. Inset: The schematic of incident light illuminating on the h-BN nanodisk. (b) Top view of the near field distribution of the normalized electric field $|E/E_0|$, 2 nm above the nanodisk at a frequency of 1444 cm^{-1}. (c) Side view of the near field distribution of the normalized electric field $|E/E_0|$ at the same frequency. The black dashed line indicates the boundary of the nanodisk. The scale bar is 10 nm.

The peak in the excitation in Fig. 3(a) originates from the LSPhP resonance and is tunable by varying the size of the h-BN disk. The extinction spectra of the h-BN disk with 2 nm thickness and different diameters are plotted in Fig. 4(a). The resonance peak position redshifts with increasing the diameter of the disk and the intensity of the extinction cross-section is proportional to the volume of the disk. According to the Frohlich condition, the resonant peaks of the h-BN disks with different diameters are calculated theoretically as shown by the dashed line in Fig. 4(b). The numerical simulation results also coincide well with the theoretical calculations, as shown

by the black dots in Fig. 4(b). The dipolar extinction of the h-BN nanodisk can be explained by the LSPhP resonance in the h-BN disk in spite of the anisotropic permittivity of h-BN. Furthermore, one can achieve the same LSPhP resonant frequency on large scale hBN disks by controlling the ratio of diameter and thickness according to the Frohlich condition.

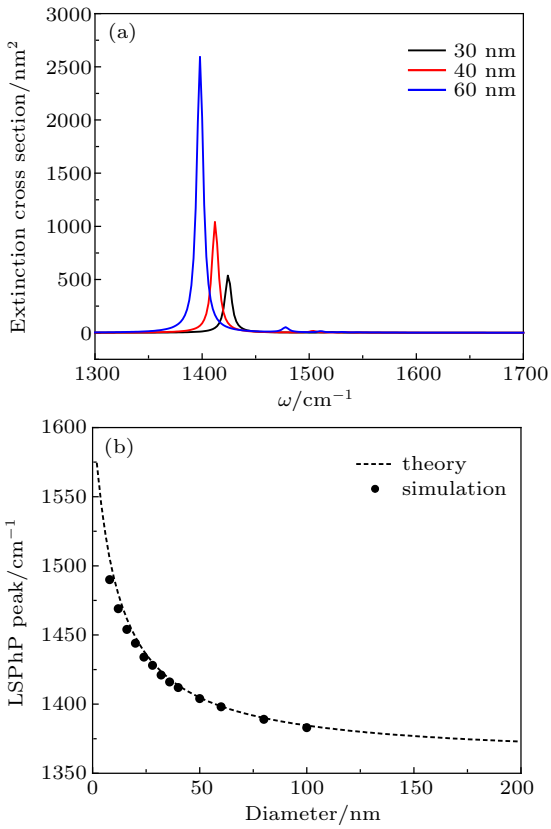


Fig. 4. Extinction spectra of h-BN disks with 2 nm thickness and different diameters of 30 nm (black line), 40 nm (red line), and 60 nm (blue line). (b) Resonance peak positions of localized surface phonon polaritons vs. the diameter of h-BN disk.

4. Conclusion

In summary, we calculate the extinction spectra of hyperbolic h-BN nanodisks, which show two origins of extinction mechanisms in the upper Reststrahlen band. The volume confined phonon polaritons propagate inside the hBN disk and exhibit Fabry–Perot resonances that lead to a series of different orders of Fabry–Perot resonant extinction peaks. The localized surface phonon polaritons in the hBN disk give rise to a significant dipolar extinction peak, and the corresponding extinction intensity is three orders stronger than that caused by the volume confined phonon polaritons. The dipolar extinction peak has a high-quality factor of 190 and an electric field enhancement factor of 40, which can be precisely tuned by the size of the hBN disk in the mid-infrared region. Our findings reveal that there are two mechanisms of extinction existing in the hBN nanodisk with distinct extinction properties, which offer a new route to manipulate light at the nanoscale, a key message for hBN based nanophotonic applications.

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