Switchable strong coupling between dual hyperbolic phonon polaritons and photons in hybrid structure of metasurfaces and h-BN slab

Meiqi Li, Qichang Ma, Aiping Luo and Weiyi Hong

Guangzhou Key Laboratory for Special Fiber Photonic Devices and Applications & Guangdong Provincial Key Laboratory of Nanophotonic Functional Materials and Devices, South China Normal University, Guangzhou 510006, People’s Republic of China

* Author to whom any correspondence should be addressed.

E-mail: hongwy@m.scnu.edu.cn

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Abstract

We propose an all-dielectric hybrid structure combined with hexagonal boron nitride slab and strontium titanate (STO) metasurfaces to excite dual hyperbolic phonon polaritons (HPhPs) and an additional optical (TO) phonon, and achieve their strong coupling with photons. The metasurfaces, supporting tunable guided-mode resonance via adjusting the external temperature, consists of STO two-dimensional grating and STO layer. Thus, the strong coupling can be switched and tuned actively between the dual HPhPs and TO phonon via adjusting the external temperature of metasurfaces. This work has numerous potential applications on multi-channel biosensors, filters and tunable source and detectors.

1. Introduction

Metasurfaces, an artificial composite material consists of sub-wavelength building blocks with small thickness, are able to support three-dimensional manipulation of light. Utilization of arrangement and interaction of basic building blocks allows for modifying the features of electromagnetic waves such as direction of propagation, and phase [1, 2]. Particularly, all-dielectric metasurfaces recently drawn numerous attentions due to low thermal conductivity and dissipation comparing metallic metasurfaces [3, 4]. The guided-mode resonance can be excited in all-dielectric metasurfaces, and shows a strong field enhancement [5]. Therefore, all-dielectric metasurfaces could provide an ideal platform for implementing enhanced light–matter interaction.

In couple system, strong coupling, as an unique regime of light–matter interaction, occurs when the rates of exchange energy between matter and photon becomes faster than the dissipation rates of other loss mechanisms. Strong coupling regime shows coherent energy oscillations (Rabi oscillations) between matter and photon, i.e., the electric field of radiation manifest a periodic beating mode at Rabi frequency in the time domain. In spectra, it results the generation of two new mixed eigenstates separated by normal mode splitting, called Rabi splitting [6, 7]. Strong coupling has huge potential applications in the fields of quantum information [8], all-optical logics [9, 10] and controlling chemical reactions and interactions. Recently, many emerging material platforms have been demonstrated to obtain strong coupling, such as topological [11, 12] and perovskite [13, 14] and semiconductor heterostructures [15, 16]. And researchers have successfully realized tunable strong coupling by using transition metal dichalcogenides materials [17, 18], phase changes materials [19] and anionic fluorescent dye [20]. However, most studies of tunable strong coupling concentrate on single-mode, hence, tunable multi-modes strong coupling still remains to be realized.

In recent years, hexagonal boron nitride (h-BN) has received extensive attentions, owing to it has potential to alternate metals to become new building blocks of nanophotonic devices in mid-infrared to THz frequencies [21, 22]. h-BN is a prototypical hyperbolic material, which exhibits anisotropic phonons
and supports hyperbolic phonon polariton (HPhP) modes [21, 23, 24]. Especially, HPhP in h-BN has extremely long lifetimes [25, 26], thus, it can be applied to strong coupling [27]. To date, the HPhP in h-BN can be excited at far-field by its manufacturing special structure, such as grating [28], ribbons [29], cones [21, 30, 31], thin flake with rectangular hole array [32] and heterostructures [33–35] or far-field Raman scattering process [36]. In addition, scanning near-field optical microscopy is used for exciting and detecting the HPhP in h-BN at near-field [25, 37]. However, until now excitation of the HPhP in h-BN slab at far-field, has remained unexplored.

Strontium titanate (STO), as an excellent phase-change materials [38, 39], its permittivity can be tuned by controlling external temperatures, which can be used for designing tunable metasurfaces [40–42]. In this work, we propose an all-dielectric hybrid structure combined with h-BN slab and all-dielectric metasurfaces to excite dual HPhPs and an additional optical (TO) phonon in h-BN slab, and achieved their switchable strong coupling with photons. For the first time to the best of our knowledge, utilizing h-BN slab at far field successfully excite HPhPs. The all-dielectric metasurfaces consist of STO rectangular bars and STO layer, therefore support the tunable guided-mode resonance due to the temperature dependence of the phase of STO. By changing the temperature, the guided-mode resonance wavelength can be tuned. Moreover, the electric field distributions \( E_z \) are analyzed to demonstrate the excitation of dual HPhPs in hybrid system. Importantly, the hybrid system can implement strong coupling at dual HPhPs modes and TO phonon by analyzing the dispersion curves and the dynamic properties of reflectivity electric field. As a result, the strong coupling can be switched and tuned actively between dual HPhPs and TO phonon by tuning temperature of metasurfaces.

2. Hybrid structure of STO metasurfaces and h-BN slab

Figure 1(a) shows the schematic of the proposed all-dielectric hybrid system, which consists of h-BN slab and all-dielectric metasurfaces. The nanostructure of the basic building block is composed of a STO rectangular bar, STO layer and h-BN layer on SiO\(_2\) substrate as illustrated in figures 1(b) and (c). The geometric parameters of the basic building block are set as: the bar with width of \( W = 360 \) nm and length of \( L = 2000 \) nm, \( h_1 \) is the thickness of the STO bar and layer, the thickness of h-BN layer is fixed as \( h_2 = 250 \) nm. The period \( P_x \) along x-axis and \( P_y \) along y-axis are fixed as 575 nm and 2500 nm, respectively.

h-BN as an anisotropic material can support two type HPhPs in the mid-infrared frequency range. Type I (\( \varepsilon_\parallel < 0, \varepsilon_\perp > 0 \)) and type II (\( \varepsilon_\parallel > 0, \varepsilon_\perp < 0 \)) HPhPs can accounts for out-of-plane (\( \omega_{\text{TO,}\parallel} = 780 \text{ cm}^{-1}, \omega_{\text{LO,}\parallel} = 830 \text{ cm}^{-1} \)) and in-plane (\( \omega_{\text{TO,}\perp} = 1370 \text{ cm}^{-1}, \omega_{\text{LO,}\perp} = 1610 \text{ cm}^{-1} \)) phonon mode, respectively. The real and imaginary part of the relative permittivity of h-BN (\( \varepsilon_\parallel = \varepsilon_{\parallel f} \) and \( \varepsilon_\perp = \varepsilon_{\perp f} \)) as shown in figure 2(a), and its dielectric function is given by [43]:

\[
\varepsilon_\xi = \varepsilon_{\infty,\xi} + \varepsilon_{\infty,\xi} \left( \frac{\omega_{\text{LO,}\xi}^2}{\omega_{\text{TO,}\xi}^2} - \frac{\omega_{\text{TO,}\xi}^2}{\omega^2} - i \omega \gamma_\xi \right), \quad \xi = \parallel, \perp
\]

where \( \varepsilon_{\infty,\parallel} = 2.95, \varepsilon_{\infty,\perp} = 4.87, \gamma_\parallel = 4 \text{ cm}^{-1}, \gamma_\perp = 5 \text{ cm}^{-1} \).

The relative permittivity of STO can be expressed as [44, 45]:

\[
\varepsilon_\omega = \varepsilon_{\infty} + \frac{f}{\omega_0^2 - \omega^2 + i \omega \gamma}
\]

where \( \varepsilon_{\infty} \approx 9.6 \) represent the high-frequency bulk permittivity, \( f \) is the temperature-dependant oscillator strength and the value is \( 2.6 \times 10^6 \text{ cm}^{-2} \), \( \omega_0 \) represent the soft mode frequency, \( \omega \) and \( \gamma \) are the frequency and soft mode damping parameter, respectively. \( \omega_0 \) and \( \gamma \) can be calculated as:

\[
\omega_0(T) \left[ \text{cm}^{-1} \right] = \sqrt{31.2(T - 42.5)}
\]

\[
\gamma(T) \left[ \text{cm}^{-1} \right] = -3.3 + 0.094T.
\]

The real and imaginary part of permittivity of the STO can be calculated by equations (2)–(4), and the results are illustrated in figure 2(b). The left and right axis represent the real and imaginary part of permittivity, respectively. By adjusting temperature, the relative dielectric constant of STO can be controlled due to temperature-dependant of \( \omega_0 \) and \( \gamma \). Thus, the STO can be applied to tunable metasurfaces.

All-dielectric metasurfaces in this work consists of STO two-dimensional grating and STO layer, which can excite a guided-mode resonance mode. Obviously, as the temperature of STO increases from 225 K to 325 K, the real and imaginary part of permittivity both decrease in figure 2(b). Meanwhile, with the increase
Figure 1. (a) Schematic diagram of the proposed all-dielectric hybrid system. (b) and (c) The top view and nanostructure of basic building block, which consists of a STO rectangular bar, STO layer and h-BN layer on SiO$_2$ substrate. The geometric parameters of the basic building block are set as: the bar with width of $W = 360$ nm and length of $L = 2000$ nm, $h_1$ is the thickness of the STO bar and layer, the thickness of h-BN layer is fixed as $h_2 = 250$ nm. The period $P_x$ along $x$-axis and $P_y$ along $y$-axis are fixed as 575 nm and 2500 nm, respectively.

Figure 2. (a) The real and imaginary part of the relative permittivity of h-BN. The color area is the hyperbolic region in RSBs, which can support type II HPhP. (b) The temperature-dependant of the relative permittivity of STO. The solid and dashed line represent the real (Re $\varepsilon$) and imaginary (Imag $\varepsilon$) part of permittivity, respectively.

of wavelength, the real part of permittivity has not significantly change, but the imaginary part of permittivity is decreasing. These result shows temperature-dependant of the relative dielectric constant of STO, hence, the guided-mode resonance of metasurfaces can be modulated via controlling the temperature ($T$) of STO two-dimensional grating and STO layer.

The COMSOL Multiphysics is employed to investigate the proposed hybrid system. The unit cell periodical boundary conditions are imposed in $x$-axis and $y$-axis directions, and the perfectly matched layers are applied in $z$-axis directions. A $x$-polarized plane wave is a normal incident.

3. Analysis

In order to illustrate the underlying mechanism of the hyperbolic photon–phonon polaritons and photon–phonon polaritons in h-BN slab and metasurfaces, the dispersion distributions of the uniform h-BN structure and the metasurfaces with h-BN slab can be derived from the imaginary part of the Fresnel reflection coefficient $r_p$. Utilizing the transfer matrix method, the complex reflectivity $r_p$ can be calculated.
Figure 3. Dispersion relation of two different structures: (a) the h-BN slab and (b)–(d) the metasurfaces with h-BN slab at STO temperatures of 300 K, 273 K and 250 K, respectively. The white dashed lines represent RSB region of h-BN.

[46]. For \( n \) layers structure, yielding the following analytical expression for \( M \):

\[
M = \begin{pmatrix}
M_{aa} & M_{ab} \\
M_{ba} & M_{bb}
\end{pmatrix} = \prod_{i=1}^{n-2} R_{i+1} \cdot T_{i+1} \cdot R_{n-1,n}.
\]

Here, \( R_{ij} \) and \( T_j \) are the boundary condition matrices and propagation matrix, respectively

\[
R_{ij} = \frac{1}{t_{ij}} \begin{pmatrix}
1 & r_{ij} \\
0 & 1
\end{pmatrix}
\]

\[
T_j = \begin{pmatrix}
e^{ik_{jz}d_j} & 0 \\
0 & e^{-ik_{jz}d_j}
\end{pmatrix}
\]

(6)

(7)

\( r_{ij} \) and \( t_{ij} \) are the Fresnel reflection, transmission coefficient for the interface between layers \( i \) and \( j \), respectively. \( k_{i,z} \) is the out-of-plane wave-vector in layer \( i \), and \( d_i \) is the thickness of layer \( i \). \( r_{ij} \) and \( t_{ij} \) can be given by:

\[
r_{ij} = \frac{\varepsilon_i k_{jz} - \varepsilon_j k_{iz}}{\varepsilon_i k_{jz} + \varepsilon_j k_{iz}}
\]

\[
t_{ij} = \frac{2\varepsilon_j k_{iz}}{\varepsilon_i k_{jz} + \varepsilon_j k_{iz}}
\]

(8)

(9)

where \( \varepsilon_j \) is the relative permittivity of layer \( i \). Finally, the complex reflectivity \( r_p \) for the \( n \) layers structure is given by a ratio of \( M_{ba} \) and \( M_{aa} \)

\[
r_p = \frac{M_{ba}}{M_{aa}}.
\]

The uniform h-BN slab structure are three layers, consisting of air/h-BN/air. Thus, the parameters used here are \( \varepsilon_1 = \varepsilon_3 = 1 \), \( \varepsilon_2 = \varepsilon_\perp \), \( k_{1,z} = k_{3,z} = \sqrt{\varepsilon_\parallel (\frac{2\pi\nu}{c})^2 - q^2} \) and \( k_{2,z} = \sqrt{\varepsilon_\perp (\frac{2\pi\nu}{c})^2 - \frac{\varepsilon_\perp}{\varepsilon_\parallel} q^2} \), where \( q \) designates the magnitude of the wavevector in the \( x-y \) plane. For the metasurfaces with h-BN slab, there are five layers, consisting of air/STO two-dimensional grating/STO/h-BN/air. The effective permittivity of two-dimensional grating for p-polarization can be calculated as [47, 48]:

\[
\varepsilon_{\text{eff},z} = \left( \frac{f_x f_y}{\varepsilon_2} - 1 - f_x f_y \frac{1}{\varepsilon_1} \right)^{-1}
\]

\[
\varepsilon_{\text{eff},x} = \left( \frac{f_x f_y}{f_y f_2} + 1 - f_x \frac{1}{\varepsilon_1} \right)^{-1}
\]

(11)

(12)
where $f_x = \frac{W}{P_x}$ and $f_y = \frac{L}{P_y}$ represent the fill factors in the $x$-axis and $y$-axis, $\varepsilon_1 = 1$ and $\varepsilon_2 = \varepsilon_{\text{STO}}$ are the relative permittivity of air and STO, respectively. The other parameters are $\varepsilon_3 = \varepsilon_{\text{STO}}, \varepsilon_4 = \varepsilon_5 = 1, k_1, z = k_5, z = \sqrt{\varepsilon_1 (2\pi\nu/c)^2 - q^2}, k_2, z = \sqrt{\varepsilon_{\text{eff}} (2\pi\nu/c)^2 - \varepsilon_{\text{eff}} q^2}$, and $k_4, z = k_{5, z} = \sqrt{\varepsilon_{\|} (2\pi\nu/c)^2 - \varepsilon_{\parallel} q^2}$.

The dispersion maps of uniform h-BN slab with the thickness $d_2 = 250$ nm, and the dispersion maps of the metasurfaces with h-BN slab at three different STO temperatures (300 K, 273 K and 250 K) can be obtained via the above calculations as depicted in figure 3. In the three the metasurfaces with h-BN slab cases, the thicknesses of STO two-dimensional grating and STO layer are set as $d_2 = d_3 = 215$ nm and the thickness of h-BN slab is $d_4 = 250$ nm. As illustrated by figure 3(a), HPhP modes are bounded inside the Reststrahlen band (RSB), and the numbers of the HPhP mode and the distributions in h-BN greatly influenced by its thickness. As shown in figures 3(b)–(d), for the metasurfaces with h-BN slab, the hyperbolic photon–phonon polaritons inside the RSB arise from the strong coupling between HPhP and photons. The photon–phonon polaritons out of the RSB is formed result of the strong coupling between photons and TO phonon polaritons. Moreover, the dispersion branch outside and inside the RSB move to higher wavelength with the STO temperatures decrease. The dispersion branch differences in the hybrid system at three different STO temperatures can be explained by temperature-dependant of the relative permittivity of STO. As the STO temperatures change, the real and imaginary part of permittivity will change so that the hybrid system is change in the energy loss.

The reflectivity spectra of metasurfaces at different temperature are illustrated in figure 4(a), where $h_1 = 215$ nm. It is shown that the resonance wavelength gradually red-shift with temperature of STO decrease. In order to investigate the metasurfaces resonance mechanism, the electric field distribution $|E|$ are calculated and presented in figure 4(b). It can be clearly observed that guided-mode resonance occurs at resonance wavelength $\lambda = 6.446 \mu$m with the typical standing wave profile. While the incident wave
diffractions in the two-dimensional grating, the wave vector can be modulated to match waveguide mode which result in the radiation of waveguide mode and guided-mode resonance can be successfully excited [5, 49–51]. In addition, the reflectivity spectra of uniform h-BN layer are shown in figure 4(c) together with the spectrum got for the metasurfaces with h-BN, where $h_1 = 180 \text{ nm}, h_2 = 250 \text{ nm} \text{ and } T = 300 \text{ K}$. The corresponding metasurfaces resonance at same parameters is shown for comparison. For uniform h-BN layer, a sharp resonance dip can be observed at $\lambda_{\text{h-BN}} = 7.333 \mu\text{m}$, which is transverse TO phonon of h-BN27. In the spectrum for the hybrid system, the dips of guided-mode resonance and h-BN transverse TO phonon and the other two dips are observed around $\lambda_{\text{M}} = 5.734 \mu\text{m}, \lambda_{\text{TO}} = 7.299 \mu\text{m}, \lambda_1 = 6.484 \mu\text{m}$ and $\lambda_2 = 6.853 \mu\text{m}$, respectively. The guided-mode resonance and TO phonon in system hybrid both occurred frequency shift comparing the uniform h-BN and metasurfaces, due to the dielectric features of the h-BN. In order to investigate the origin of the two dips ($\lambda_1$ and $\lambda_2$), the electric field distributions $E_z$ at $\lambda_1$ and $\lambda_2$ are simulated in figures 4(d) and (e). Notably, the fields exhibit a ‘zigzag’ polaritonic rays pattern inside the h-BN layer ($x$–$z$ plane), which is a feature of HPhP and demonstrate the excitation of dual HPhPs in hybrid system [25, 32, 37]. For the convenience of analysis, dual HPhPs mode are defined as HPhP I ($\lambda_I$) and HPhP II ($\lambda_{\text{II}}$), respectively. When metasurfaces resonance $\lambda_{\text{M}}$ is tuned at $\lambda_1, \lambda_2$ or $\lambda_{\text{TO}}$, the hybrid system implement strong coupling and energy oscillates between the dual HPhPs or TO phonon and the electromagnetic filed, respectively. Meanwhile, the periodic energy transfer (Rabi oscillations) happens at Rabi frequencies.

In order to verify strong coupling between the three modes (dual HPhPs and TO phonon) and the photons, the reflectivity spectra of hybrid system with different resonance wavelength of metasurfaces are simulated, where temperature of STO is $T = 300 \text{ K}$. In figures 5(a)–(c), the metasurfaces resonance is tuned from 5.974 $\mu\text{m}$ to 7.901 $\mu\text{m}$ by varying the thickness of metasurfaces $h_1$ from 194 nm to 312 nm, where the $x$-axis and $y$-axis represent metasurfaces resonance and the spectra, respectively. The anti-crossing behavior as hallmark of strong coupling can be observed from the two polaritonic branches around $\lambda_1, \lambda_{\text{II}}$ and $\lambda_{\text{TO}}$ in figures 5(a)–(c). Moreover, the two polaritonic branches converge nicely toward the $\lambda_1, \lambda_{\text{II}}$ and $\lambda_{\text{TO}}$, which mean the anti-crossing wavelengths approach the $\lambda_1, \lambda_{\text{II}}$ and $\lambda_{\text{TO}}$. With the resonance wavelength of

![Figure 5](image-url)
metasurfaces increase, the photons mode successively coupled with the HPhP I, HPhP II and TO phonon modes, and two hybrid modes can be noticed from all reflectivity spectra in figures 5(d)–(f). The spectral positions and strength of two hybrid modes are modified by the detuning between the three modes (dual HPhPs and TO phonon) and the photons. At zero-detuning, the two hybrid modes exhibit distinct anti-crossing behavior and the Rabi splitting can be observed.

Furthermore, the dynamic properties of Rabi oscillations are investigated to further verify the hybrid system implement strong coupling. In this part, the $T$ is fixed as 300 K. Three mid-infrared ultrafast Gaussian pulse (0.5 ps, 1.50 ps and 1.30 ps pulse width), respectively tuned to anti-crossing wavelengths $\lambda_I = 6.484 \mu m$ ($h_1 = 215 \text{ nm}$), $\lambda_{II} = 6.853 \mu m$ ($h_1 = 237 \text{ nm}$) and $\lambda_{TO} = 7.299 \mu m$ ($h_1 = 260 \text{ nm}$), are used for simultaneously exciting the one mode of the HPhPs and TO phonon of h-BN layer and photons mode of metasurfaces. In this case, the rates of exchange energy between the three modes (dual HPhPs and TO phonon) and the photons becomes faster than the dissipation rates of other loss mechanisms, which resulting in periodic energy transfer between the h-BN layer and the metasurfaces. Therefore, the electric field of radiation manifest a periodic beating mode at Rabi frequency in the time domain. As depicted in figures 6(a)–(c), the time evolution of reflectivity pulses of coupled system exhibit oscillations behavior with periods of 1.00 ps, 3.75 ps and 4.50 ps, respectively. These oscillations are Rabi oscillations and directly reflect the periodic energy transfer between the three modes (dual HPhPs and TO phonon) and the photons, which demonstrate the features of strong coupling in time-domain [6, 7, 15].

On the other hand, the switchability of strong coupling modes can be realized, due to metasurfaces resonance wavelength can be tuned via controlling the temperature of STO bars and layer. Figure 6(d) shows the reflectivity spectra of the proposed hybrid system at different temperatures of STO bars and layer. With the temperature decrease from 300 K to 250 K, the metasurfaces resonance wavelength red-shifts, and the hybrid system achieved the strong coupling at $\lambda_I$ ($T = 300 \text{ K}$), $\lambda_{II}$ ($T = 273 \text{ K}$) and $\lambda_{TO}$ ($T = 250 \text{ K}$) in turn. Therefore, strong coupling can be switched and tuned actively between dual HPhPs and TO phonon by selecting the corresponding temperature.

4. Conclusions

In conclusion, an all-dielectric hybrid structure with STO two-dimensional grating, STO layer and h-BN slab is proposed and demonstrated to implement the switchability of strong coupling between dual HPhPs (and an additional TO phonon) and the photons. The all-dielectric metasurfaces supporting guided-mode resonance consists of STO two-dimensional grating and STO layer. The dispersion relations are analyzed to demonstrated the all-dielectric metasurfaces with h-BN slab at different STO temperatures can support hyperbolic photon–phonon polaritons inside RSB region and photon–phonon polaritons outside of the RSB region. The guided-mode resonance wavelength can be tuned via controlling the temperature of STO.
two-dimensional grating and layer. In addition, the TO phonon is obtained in uniform h-BN slab. The result of electric field distribution $E_z$ demonstrates the excitation of dual HPhPs in hybrid system. Moreover, the dispersion curves and the dynamic properties of reflectivity electric field both confirm the all-dielectric hybrid system can implement strong coupling at dual HPhPs and TO phonon mode. Consequently, owing to the tunability of guided-mode resonance, the strong coupling can be switched and tuned actively between the three modes (HPhP I, HPhP II and TO phonon) and photons via selecting the corresponding temperature. The proposed all-dielectric hybrid system has numerous potential applications on multi-channel biosensors, filters and tunable source and detectors.

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**Disclosures**

The authors declare no conflicts of interest.

**Data availability statement**

The data that support the findings of this study are available upon reasonable request from the authors.

**ORCID iDs**

Wei yi Hong [https://orcid.org/0000-0001-6262-1070](https://orcid.org/0000-0001-6262-1070)

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