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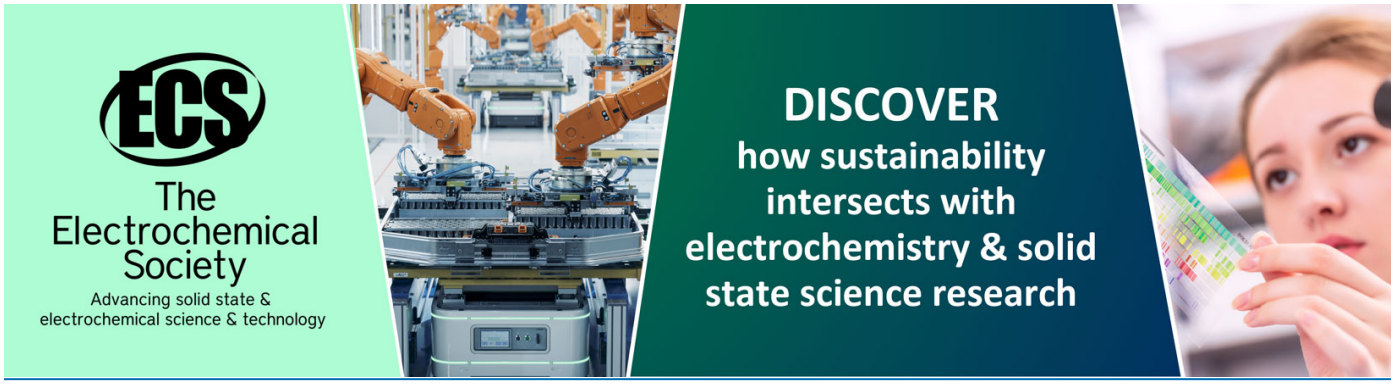

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Strong coupling of phonon polaritons in h-BN nanowires with graphene plasmons

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Abstract. The phonon polaritons in hexagonal boron nitride (h-BN) can couple with graphene plasmons, forming new hybrid modes which are called plasmon-phonon polaritons. In this paper, we point out that such coupling can occur within the strong coupling regime, where the dispersion relations of the graphene plasmons and the phonon polaritons avoid crossing with each other. We have investigated graphene-wrapped h-BN nanowires, and found that such strong couplings exist between the graphene plasmons and the fundamental as well as the high-order phonon polariton modes, even if the graphene layer is far away from the h-BN. This is interesting because the high-order phonon polariton modes are mostly confined within the bulk h-BN with little fields outside the nanowire, i.e., the interactions of these modes with the graphene plasmons should be rather weak; however, our calculations disagree with such judgements. Due to the dispersive permittivity of h-BN, the graphene plasmons can couple simultaneously with two branches of phonon polariton modes under carefully chosen electron doping levels. Our investigations may open the way to explore the plasmon-phonon polaritons in the strong coupling regime.

1. Introduction

The phonon resonances in the material may lead to negative permittivity components in the dielectric tensor, creating so-called hyperbolic materials [1]. Hexagonal boron nitride (h-BN) is such a material, which has two active infrared phonon modes: out-of-plane A_{2u} phonon mode, enabling type I hyperbolic response; and in-plane E_{1u} phonon mode, enabling type II hyperbolic responses [2,3]. Compared with artificial hyperbolic metamaterials, which often suffer from ohmic losses and low-yield fabrication processes, these naturally formed hyperbolic materials may be more useful for applications in infrared photonic devices, such as superlens and waveguides [3-5].

Despite that h-BN supports low-loss surface phonon polariton modes in the mid-infrared region, its phonon resonances are intrinsic properties of the material; thus, they are not tunable by external fields. Recently, h-BN graphene heterojunctions have been proposed which support plasmon-phonon polaritons [6,7]. These hybrid modes possess low propagation losses while maintaining tunable through the fermi level of graphene, providing a promising platform for low-loss mid-infrared nanophotonic applications. In this paper, we investigate the forming of these hybrid modes in the strong coupling regime, which is often ignored by other researchers, but indeed can occur once the graphene is separated from the bulk h-BN with a moderate gap. Our investigations may open the way to explore the plasmon-phonon polaritons in the strong coupling regime.

2. Phonon polaritons in h-BN nanowires

We analytically calculated the transverse magnetic (TM) polarized phonon polariton modes in h-BN nanowires. Naturally grown h-BN nanowires have lattice structures which can be seen as constructed by rolling up the planar boron nitride sheets into a cylinder. Due to the existence of the in-plane E_{1u} phonon mode, the effective permittivity within the boron nitride plane is negative, which makes h-BN similar to metallic materials. After the rolling, the nanowire of course possesses negative permittivities along the axial and azimuthal directions.

2.1. Theoretical model

H-BN is an anisotropic material. In the upper Reststrahlen band, the nanowire has positive permittivity along the radial direction, but negative permittivities along the axial and azimuthal directions. Thus, in order to find the phonon polariton modes, h-BN nanowires must be treated as anisotropic waveguides. Under the cylindrical coordinates, the permittivities along the axial, radial and azimuthal directions are respectively denoted as ε_z, ε_r and ε_θ. The TM-polarized modes have electric field component E_z and E_r, and magnetic field component H_θ in the cylindrical coordinates; from the mode electric field components, we can expect that the dispersion relations depend on both the radial and axial permittivities. After matching the boundary conditions, the dispersion relations of the TM-polarized phonon polariton modes are found to be determined by the following equations:

$$0 = \left[\alpha_1 {k_r}^1 \frac{\mathrm{I}_1({k_r}^1 R)}{\mathrm{I}_0({k_r}^1 R)} + \alpha_2 {k_r}^2 \frac{\mathrm{K}_1({k_r}^2 R)}{\mathrm{K}_0({k_r}^2 R)} \right] \tag{1}$$

where $\alpha_i = k_0 {\varepsilon_r}^i / (k_z^2 - {\varepsilon_r}^i k_0^2)$, ${k_r}^i = \sqrt{{\varepsilon_z}^i (k_z^2 - {\varepsilon_r}^i k_0^2) / {\varepsilon_r}^i}$ (i = 1 or 2, respectively corresponding to the region inside and outside the nanowire). I_0 and K_0 are the modified Bessel functions of the first and the second kind, respectively. Using Equation 1, we can simultaneously determine the real and the imaginary parts of the mode propagation constant accurately.

2.2. Phonon polaritons in h-BN nanowires

After tedious calculations, we have derived the TM-polarized phonon polariton modes in a h-BN nanowire with a radius of 100 nm, as shown in Figure 1. As one can see, multiple modes are found. Both the real and the imaginary parts of the mode propagation constants are derived, as shown by the solid and dashed curves in Figure 1(a), respectively. Only the first three modes are plotted, TM_0, TM_1 and TM_2, denoted by black red and blue curves, respectively. The subscripts indicate the number of the nodes of the field component E_z along the radial direction. The pink line in Figure 1(a) is the light line; thus, the phonon polariton modes in the h-BN nanowire are extremely dispersive, which of course caused by the permittivities of h-BN in the upper Reststrahlen band.

Due to the fact that h-BN is a natural hyperbolic material, the h-BN nanowire supports multiple TM-polarized phonon polariton modes; all of them are propagative modes, with the fields deeply confined within the bulk material. The normalized electric field distributions of the TM_0, TM_1 and TM_2 modes are shown in Figures 1(b), 1(c) and 1(d), respectively. The TM_0 mode has most of the electric fields confined around the surface, while the TM_1 and TM_2 modes have electric fields that are mostly confined within the bulk material. Such different field distributions may lead to the conclusion that the TM_0 mode may have strong couplings with the surroundings, while the high-order ones do not. However, our calculations strongly disagree with such conclusion, and show that the high-order phonon polariton modes can have ultra-strong couplings with other fundamental excitations. The physical reason for this is quite simple: high-order phonon polaritons have mode profiles with mostly fields within the material, while other excitations such as plasmons may possess extensive field distributions which may cause large field overlaps with the high-order phonon polariton modes; thus, strong couplings can still exist. In the followings, we analytically investigate such couplings within the framework of electrodynamics.

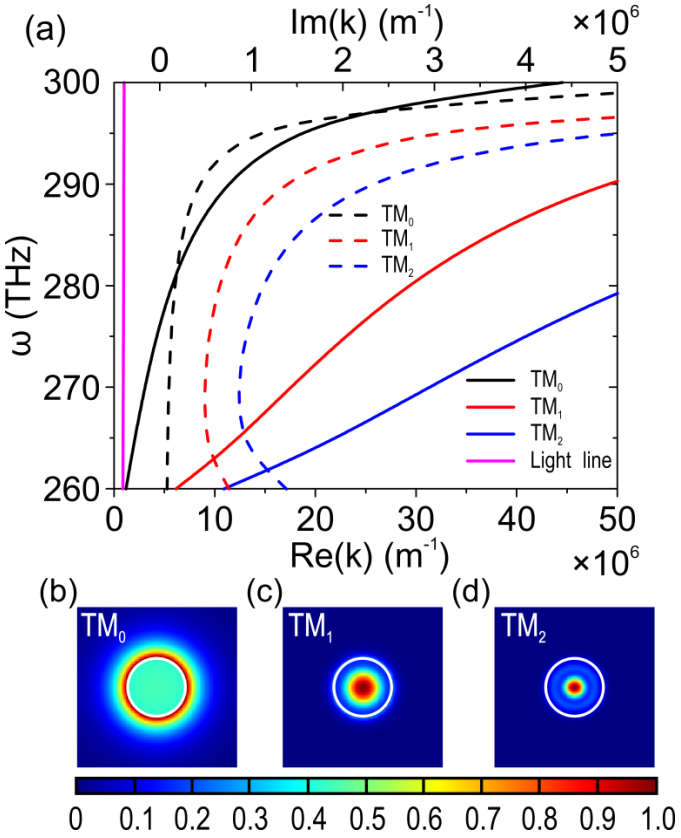

Figure 1. (a) Phonon polariton modes in the h-BN nanowire with a radius of 100nm. The normalized electric field distributions of the (b) TM_0, (c) TM_1, and (d) TM_2 modes.

3. Plasmon-phonon polaritons in the strong coupling regime

In the upper Reststrahlen band, h-BN supports TM-polarized phonon polariton modes. Since graphene plasmons are also TM-polarized, couplings between these two kinds of polaritons are possible. The graphene-wrapped h-BN nanowire is investigated in this paper as an analytic model for deriving the plasmon-phonon polaritons in the strong coupling regime, as schematically shown in Figure 2.

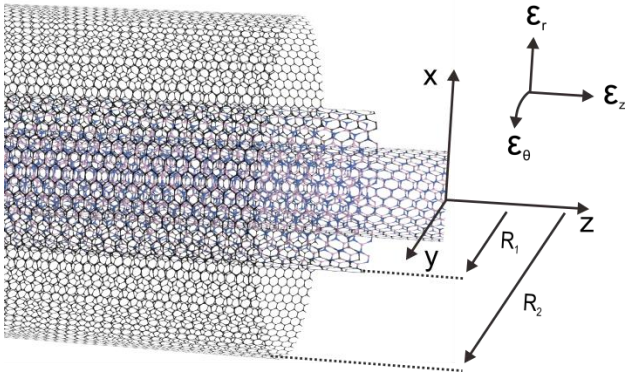

Figure 2. Schematic of the graphene-wrapped h-BN nanowire, where the propagation is along the *z*-axis. Graphene sheet is also rolled up into a cylinder, indicated by the large black tube with a radius of R_2, and the h-BN nanowire has a radius of R_1.

H-BN nanowire forms the core of the system, which has a radius of R_1; graphene layer is rolled up in to a cylinder, which has a radius of R_2. In this paper, we have $R_2 \geq R_1$. The permittivities along the radial, azimuthal and axial directions are respectively denoted as ε_r, ε_θ and ε_z. Given the lattice structures, we have $\varepsilon_\theta = \varepsilon_z = \varepsilon_{//}$ and $\varepsilon_r = \varepsilon_\perp$, where $\varepsilon_{//}$ and $\varepsilon_\perp$ are the permittivities parallel and perpendicular to the c-axis of h-BN [2-4]. In the calculations, the permittivities of the bulk h-BN were used; the TM-polarized plasmon-phonon polaritons were determined using the waveguide theory. After matching the boundary conditions, we have derived a determinant:

$$\begin{vmatrix} \mathrm{I}_0(a) & -\mathrm{I}_0(b) & -\mathrm{K}_0(b) & 0 \\ 0 & \mathrm{I}_0(c) & \mathrm{K}_0(c) & -\mathrm{K}_0(d) \\ -i\beta_1 \mathrm{I}'_0(a) & i\beta_2 \mathrm{I}'_0(b) & i\beta_2 \mathrm{K}'_0(b) & 0 \\ 0 & i\beta_2 \mathrm{I}'_0(c) - \gamma \mathrm{I}_0(c) & i\beta_2 \mathrm{K}'_0(c) - \gamma \mathrm{K}_0(c) & -i\beta_3 \mathrm{K}'_0(d) - \gamma \mathrm{K}_0(d) \end{vmatrix} = 0 \quad (2)$$

where $\gamma = Z_0\sigma / 2$ and $\beta_i = \alpha k_{ri}$ (i = 1, 2, 3. The h-BN core, the space outside graphene and the volume between them are respectively denoted by i = 1, i = 3, and i = 2.). Z_0 is the vacuum impedance and σ is the graphene conductivity. Letters *a, b, c and d* respectively denote $k_{r1}R_1$, $k_{r2}R_1$, $k_{r2}R_2$ and $k_{r3}R_2$. Other letters have the same meanings as in Equation (1). In this paper, graphene has been treated as a curved conductive surface. Using Equation 2, the dispersion relations can be determined. We chose R_1 = 100 nm, R_2 = 200 nm. The fermi level of graphene can be varied, modifying the coupling strength between the phonon polaritons and the graphene plasmons.

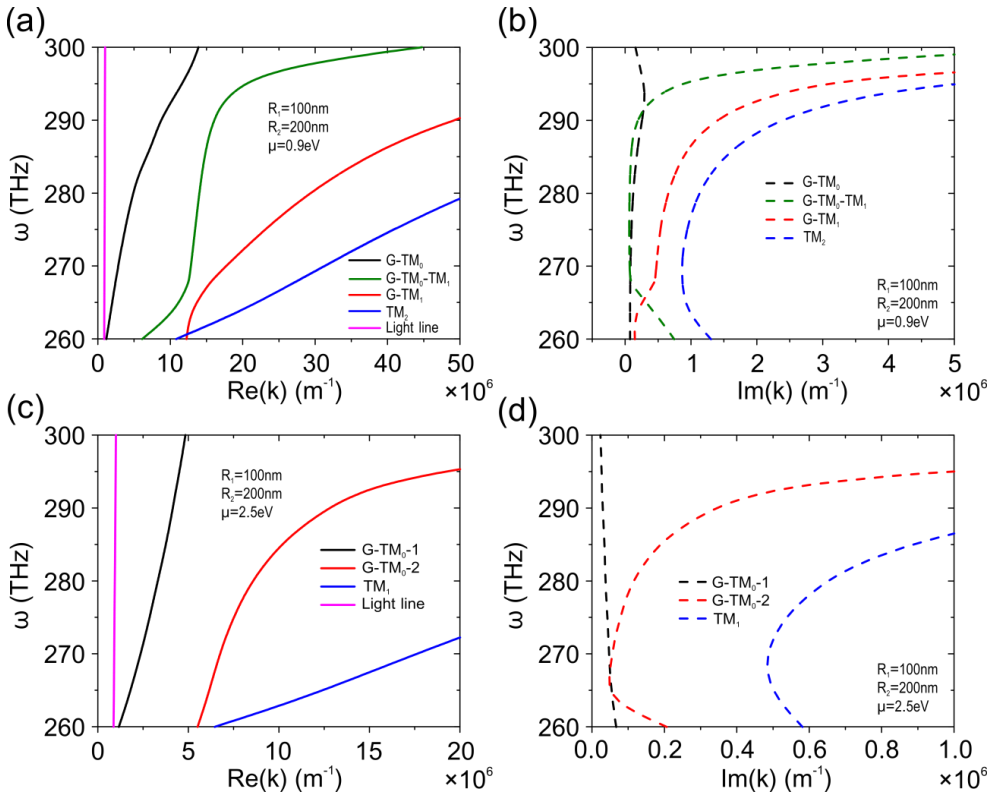

Figure 3. (a) The dispersion relations of the plasmon-phonon polariton modes when μ = 0.9 eV. (b) The corresponding imaginary parts of the modes in (a). (c) The dispersion relations of the plasmon-phonon polariton modes when μ = 2.5 eV. (d) The corresponding imaginary parts of the modes in (c).

Figures 3(a) and 3(b) respectively show the real and the imaginary parts of the propagation constants of the hybrid plasmon-phonon polaritons modes under the condition of μ = 0.9 eV; Figures 3(c) and 3(d) respectively show the real and the imaginary parts of the propagation constants of the hybrid plasmon-phonon polaritons modes under the condition of μ = 2.5 eV. With μ = 0.9 eV, the dispersion relation of the graphene plasmons, denoted as G, simultaneously across with the TM_0 and TM_1 phonon polariton modes in h-BN nanowire, as shown in Figure 3(a), indicating two couplings: one is near 295 THz, forming the G-TM_0 plasmon-phonon polariton mode, denoted by the black curve; the other is near 265 THz, forming the G-TM_1 plasmon-phonon polariton mode, denoted by the red curve. The green curve in Figure 3(a) originates from the graphene plasmons; however, due to the mode coupling, it shows three distinct sections: the first one is below 265 THz; the second one is from 265 THz to 295 THz; the third one is above 295 THz. The first and the third sections are phonon-like, while the second section is plasmon-like. We come to these conclusions based on the slopes of the dispersion curves in three sections. The corresponding imaginary parts of the propagation constants (denoted as Im(k)) are plotted in Figure 3(b). At the coupling frequencies, their imaginary parts across with each other, showing totally different phenomena from Figure 3(a). With μ = 2.5 eV, the dispersion relation of the graphene plasmons, denoted as G, only across with the TM_0 phonon polariton mode, causing only one coupling near 265 THz, as shown in Figures 3(c) and 3(d), forming two hybrid plasmon-phonon polariton modes, respectively denoted as G-TM_0-1 and G-TM_0-2. One can see that the high-order phonon polariton modes, like TM_1, are still important, since they can have strong couplings with other excitations, for example graphene plasmons. TM_2 and even higher order phonon polariton modes may also have such strong couplings, depending on the configuration of the composite systems.

4. Conclusion

In our paper, we show that the plasmon-phonon polaritons in graphene and h-BN composite structures can be formed in the strong coupling regime. The high-order phonon polariton modes in h-BN nanowires are still important due to the possibility of their strong couplings with other fundamental excitations, for example, plasmons. Due to the dispersive permittivity of h-BN, such strong coupling can occur simultaneously in two branches of phonon polaritons, depending on the parameters of the graphene. Our investigations may lead to the exploration of plasmon-phonon polaritons in graphene and h-BN composite structures within the strong coupling regime.

Acknowledgments

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