A systematic insight into the surface plasmon polaritons guided by the graphene based heterostructures

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Abstract: Graphene paves the way for the outstanding applications as it is one-atom thick and possesses perfect tunability properties. The main goal of this work is to study mode patterns of surface waves propagating in the graphene-based structures in the far-infrared region. Herein, we study a broad variety of graphene structures starting with the simplest graphene/dielectric interface guiding conventional surface plasmon polaritons (SPPs) and ending up with more complicated cases allowing to have a deeper insight into the complexity of the mode patterns tunability features provided by graphene paving the way for the hybridized waves. Thus, the hybridized surface-phonon-plasmon-polaritons (SPPPs) guided by graphene/LiF/glass compounds are theoretically studied. By constructing a heterostructure comprising graphene and LiF one may benefit from the advantages of both, resulting in engineerable hybridized SPPPs propagating in both directions, i. e. either forwardly or backwardly. Moreover, we conclude with presentation of the metamaterial composed of graphene and LiF building blocks allowing for an enhanced degree of freedom.

1. Introduction

Graphene, treated as a two-dimensional (2D) form of carbon with the atoms organized in a honeycomb lattice [1, 2], has attracted tremendous attention so far due to its outstanding mechanical, electric, magnetic and thermal characteristics paving a way for a large stream of exciting applications that are being vigorously pursued by academia and industry [3].

A way to achieve simultaneous subdiffractional confinement through the stimulation of surface phonon polariton (SPhP) modes [4] is also offered by polar dielectrics alongside noble metals and graphene. SPhPs appear because of the interaction of optical phonons with long-wavelength incident fields. The former phenomenon creates a surface excitation mediated by the atomic vibrations. One can stimulate such SPhP modes between the longitudinal optical (LO) and transverse optical (TO) phonon frequencies of the polar dielectrics. This spectral range is named as the Reststrahlen (RS) band or polaritonic gap. Because of appearance of SPhPs, polar-based metamaterials fit perfectly well for light absorption and coherent thermal emission in the mid- and far-IR ranges [4].

The first optical investigations of graphene plasmons have been conducted in the terahertz frequency range [5]. Some time before, terahertz and far-infrared measurements of terahertz plasmons in traditional 2D electron gas were extensively performed [6-8]. To get a deeper insight into the problem, it is very natural to expand these investigations to a comparatively new 2D electron gas system (i.e. graphene). However, this is not a simple replica of the previous effort. Graphene terahertz plasmon paves a way for a large stream of possible applications.

Herein, we provide a systematic insight into the mode patterns tunability features possible due to the inclusion of a graphene layer into the structure under consideration. We start an analysis from the simplest case, i. e. graphene/dielectric interface for guiding conventional surface plasmon polaritons (SPPs). Then, we proceed with investigating of the graphene heterostructure constructed by employing graphene and dielectric layers. To have a deeper insight into the SPhP modes, we study dispersion of surface-phonon-plasmon-polaritons (SPPPs) guided by the graphene layer deposited on a LiF film [9, 10], a polar dielectric. We report on the SPhPs guided by thin films of LiF. We will have a deeper insight into the dispersion of highly confined and long-range phononic modes propagating in a 10 nm thick LiF waveguide on glass substrate at 10-18 THz. Moreover, graphene layer and LiF film will be combined in one compound aiming to benefit from tunability and wide-range variations of permittivity. Dispersion of SPPPs of this heterostructure will be studied. We will demonstrate that the region of LiF with high permittivity values can make a positive impact on the SPPPs dispersion below the polaritonic gap. The former is consistent with the results for SPPs, obtained in the case of dispersion-free lossless substrates. To finalize an analysis we will combine graphene and LiF in one metamaterial structure aiming to obtain SPPs with the enhanced properties with a degree of freedom.

2. Results and Discussion

Model of graphene

The optical conductivity of graphene ($\sigma_g = \sigma_g^{intra} + \sigma_g^{inter}$) can be expressed as follows [11]

$$\sigma_g^{intra} = \frac{e^2}{4\hbar}\frac{i}{2\pi}\left\{\frac{16k_BT}{\hbar\Omega}\ln\left(2\cosh\left(\frac{\mu}{2k_BT}\right)\right)\right\} \tag{1}$$

$$\sigma_g^{inter} = \frac{e^2}{4\hbar}\left\{\frac{1}{2}+\frac{1}{\pi}\arctan\left(\frac{\hbar\Omega-2\mu}{2k_BT}\right)-\frac{i}{2\pi}\ln\frac{(\hbar\Omega+2\mu)^2}{(\hbar\Omega-2\mu)^2+(2k_BT)^2}\right\} \tag{2}$$

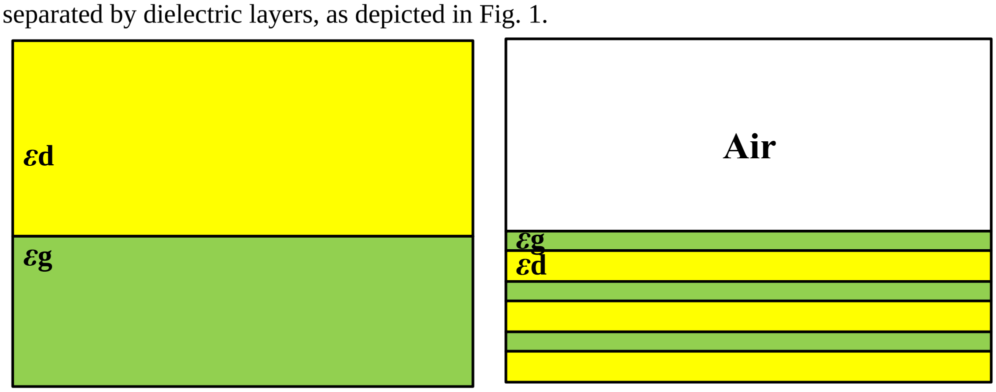
With $\Omega = \omega + i\tau^{-1}$, μ is chemical potential of graphene, e is the electron charge, k_B is the Boltzmann constant, $\hbar$ is the Plank constant over 2π, and c is the speed of light in vacuum. Herein $\tau = 0.2\,ps$ and T=300 K.

SPPs of graphene heterostructures

Let us start with the fundamental equation governing the complex wavevectors of SPP stated here for the convenience [12]:

$$\beta = \sqrt{\frac{\varepsilon_g\varepsilon_d}{\varepsilon_g+\varepsilon_d}}k \tag{3}$$

β is the complex wavevector of the SPPs propagating at the graphene/dielectric interface.
Let us consider hyperbolic metamaterial heterostructures made of stacked graphene sheets separated by dielectric layers, as depicted in Fig. 1.



(a) (b)

Fig. 1. Schematic view of graphene/dielectric interface (a) and an interface separating infinite layered nanoctructured metamaterial formed by alternating graphene and dielectric layers and air (b).

The effective-medium approach which is justified if the wavelength of the radiation considered is much larger than the thickness of any layer is applied aiming to describe the optical response of such a system (Fig. 1(b)). The former is based on homogenization the structure parameters. Thus, further in this section the effective homogeneous media for two semi-infinite periodic structures is considered. The effective permittivities are as follows [13]:

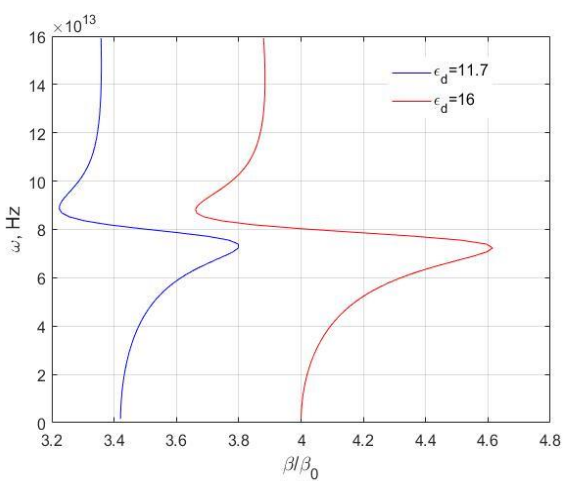
$$\varepsilon_{\parallel} = \frac{\varepsilon_g d_g + \varepsilon_d d_d}{d_g + d_d} \tag{4}$$

$$\varepsilon_{\perp} = \frac{\varepsilon_g \varepsilon_d \left(d_g + d_d\right)}{\varepsilon_g d_d + \varepsilon_d d_g}, \tag{5}$$

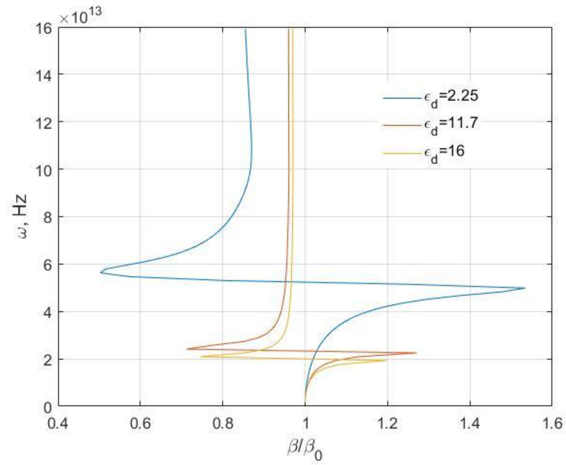
Matching the tangential components of the electrical and magnetic fields at the interface results in the dispersion relation for the surface modes localized at the boundary separating two media. It is assumed that the permittivity of graphene $\varepsilon_g\left(\omega\right)$ is frequency dependent. The effective permittivity ε_g of graphene can be determined as follows [14]: $\varepsilon_g = 1 + i\sigma / \varepsilon_0 \omega d_g$, where d_g is the thickness of graphene sheet, ε_0 is the permittivity in the vacuum.

It is worthwhile noting, that one can dramatically control the frequency range of the surface wave existence by modifying the permittivities and thicknesses of the layers [15] employed in the nanostructured metamaterial (Fig. 1(b)). It is of particular importance to evaluate the tangential components of the electric and magnetic fields at the interface and obtain a single surface mode with the propagation constant seeking to get the unique dispersion relation for the surface modes confined at the metamaterial/air interface [16].

$$\beta = k\sqrt{\frac{\left(1-\varepsilon_{\parallel}\right)\varepsilon_{\perp}}{1-\varepsilon_{\perp}\varepsilon_{\parallel}}}, \tag{6}$$



(a)



(b)

Fig. 2. Dispersion supported by a graphene/dielectric interface (a) and by graphene heterostructure (b).

It should be stressed, that application of the dielectric substrate has a pivoting role seeking for a feasible design. Also, it enables advances physical regimes and operating modes. One may effectively control various electromagnetic phenomena by a proper choice of substrate [17-21]. By properly modifying the substrate, the same characteristics can be obtained at different frequency ranges by mimicking their properties. The conventional scaling tule of resonance frequencies, $f \propto \varepsilon_d^{-1/2}$ (ε_d is permittivity of dielectric filling a cavity), is known for lossless cavities. However, one may hardly predict scaling performance for an open resonance structure. The former takes place as identification of the predetermined boundary of the region occupied by the resonance field stands for as the challenging task. A proportional change of both geometrical and material properties opens the wide avenues for scaling of the current transmittive/reflective structure with respect to frequency. Moreover, one may seek for a partial scaling by engineering dielectric properties of substrate. In this case all geometrical dimensions are treated as constant values. Moreover, effect of dielectric substrate on nature of plasmons in silver nanowires makes a dramatic impact on the system properties [22]. Naturally, downscaling (for fixed frequency) or redshift (for fixed geometry) is caused by the increase of permittivity. Though, aiming to quantify these effects one needs to apply a detailed numerical study.

Herein, the impact of various, dispersion-free lossless substrates on the properties of graphene SPPs is examined. The considered substrates include Si, Ge (Fig. 2(a)). One may observe in Fig. 2(a) that increase of ε_d leads to graphene SPPs supported for larger values of the wavenumber at fixed frequencies. Doing so, SPPs can propagate with smaller λ_{sp} and group velocity, v_g. Changes of ε_d in graphene-based metamaterial allow for the tunability features of dispersion diagrams (Fig. 2(b)). Doing so, one may increase the range of the surface waves existence. The scaling is appropriate to the results depicted in Fig. 2. Doing so, one may introduce $\varepsilon_d^{-1/2}$ -like fitting in the same way as in [21].

SPhPs of LiF heterostructures

Dispersion-free materials possessing high permittivity values do not exist in the far-IR. Consequently, the former may lead to the choice of polar dielectrics like LiF, NaCl, and GaAs.

These materials are known to exhibit a polaritonic gap (RS band). The former phenomenon takes place because of the phonon-photon interaction. This interaction provides anticipated high permittivity values. One may witness the hybridization of SPPs with phonons at the far-IR if the heterostructures constructed out of graphene and polar materials. Having in mind the fabrication purposes, those materials should be used as a buffer layer between a single-layer graphene and a thicker low-loss dielectric substrate. In this relation, one has to study the waveguide structures made of thin films of a polar dielectric on low-loss dielectric substrate before proceeding with combining with graphene. Herein, we examine dispersion properties of SPhPs guided by thin films of LiF on different lossless substrates. LiF suits perfectly well for these purposes due to its wide RS band and opportunities to engineer permittivity inside and around this band.

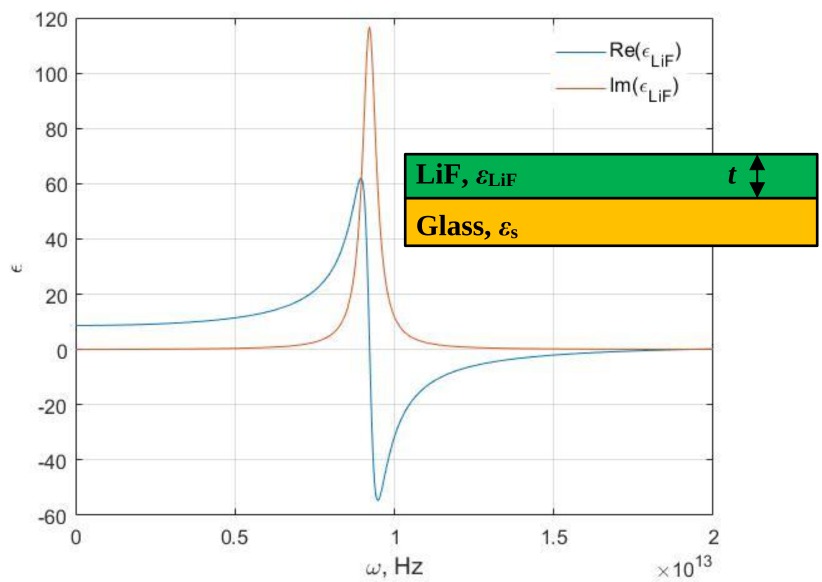


Figure 3. Permittivity of LiF $\varepsilon_{\mathrm{LiF}}$ within 1-20 THz. Real part is depicted by the solid blue line, imaginary part – by the solid red line.

A LiF film sandwiched on the top of a substrate with ε_{s} is schematically demonstrated in the inset of Fig. 3. The LiF under consideration is characterized by the thickness *t* and permittivity expressed as follows [23]:

$$\varepsilon_{LiF} = \varepsilon_{\infty}\left(1 - \frac{\omega_{LO}^2 - \omega_{TO}^2}{\omega^2 - \omega_{TO}^2 - i\gamma\omega}\right) \tag{7}$$

where $\varepsilon_{\infty} = 2.027$, $\omega_{TO} = 2 f_{TO}$, $\omega_{LO} = 2 f_{LO}$, $f_{TO} = 9.22 THz$, $f_{LO} = 19.1 THz$ and $\gamma = 2\pi \times 0.527 THz$. Here, f_{TO}, f_{LO} and γ are, respectively, transverse optical frequency, longitudinal optical frequency and damping factor. Fig. 3 presents real and imaginary parts of $\varepsilon_{\mathrm{LiF}}$. One may conclude with the following dispersion relation of the SPhPs that are guided by the LiF layer placed on the dielectric substrate [23]:

$$\tanh\left(q_{LiF}t\right) = -\frac{\varepsilon_{LiF} q_{LiF}\left(\varepsilon_s q_a + \varepsilon_a q_s\right)}{q_a q_s \varepsilon_{LiF}^2 + \varepsilon_a \varepsilon_s q_{LiF}^2}, \tag{8}$$

Where $q_{LiF} = \sqrt{\beta^2 - \varepsilon_{LiF}\beta_0^2}$, $q_a = \sqrt{\beta^2 - \varepsilon_a\beta_0^2}$, $q_s = \sqrt{\beta^2 - \varepsilon_s\beta_0^2}$.

Dispersion of the SPhPs for the LiF layer sandwiched on different substrates is investigated. Fig. 4 demonstrates the obtained results. One may conclude from Fig. 4 that SPhPs are guided in the polaritonic gap (RS band) on LiF, in which $\mathrm{Re}\left(\varepsilon_{LiF}\right) < 0$.

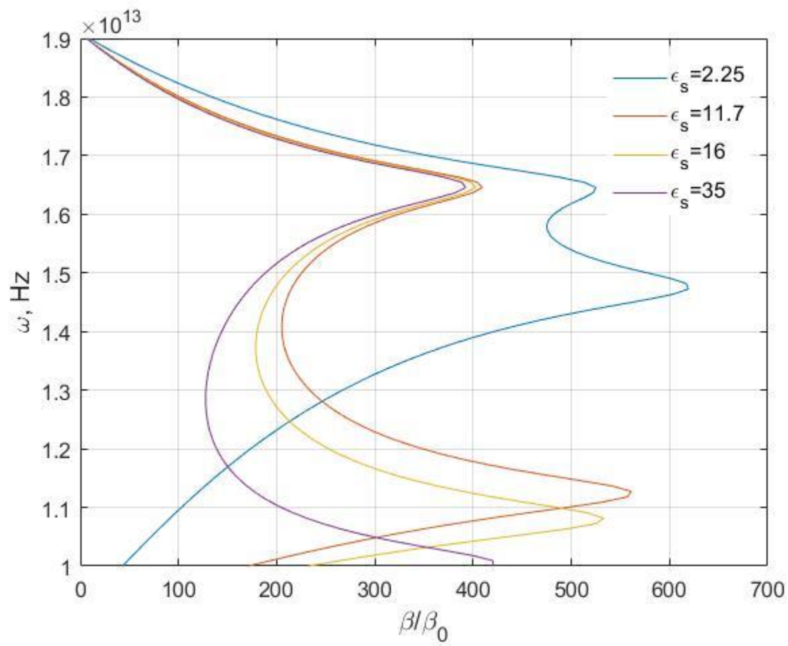


Figure 4. Dispersion of waves guided by air/LiF waveguides of thickness *t* positioned on a dielectric substrate.

To have a deeper insight into graphene based heterostructures, graphene and LiF are combined in one hybrid structure aiming to benefit from engineerable properties of graphene and a wide permittivity range of LiF. Doing so, graphene SPPs could be hybridized with SPhPs. The structure depicted in Fig. 3 is enhanced by sandwiching a single layer of graphene positioned on top of the LiF film. It is illustrated in the inset of Fig. 5. Making a certain kind of rearrangements the dispersion equation of the coupled plasmonic-phononic modes of this structure is obtained [23]

$$\tanh\left(q_{LiF}t\right) = -\frac{\varepsilon_{LiF} q_{LiF}\left(\varepsilon_s q_a + \varepsilon_a q_s - \alpha q_a q_s\right)}{\varepsilon_{LiF}^2 q_a q_s + \varepsilon_a \varepsilon_s q_{LiF}^2 - \alpha \varepsilon_s q_{LiF}^2 q_a} \tag{9}$$

where $\alpha = \sigma_g / i\omega\varepsilon_0$. The former are labeled as surface-phonon-plasmon-polaritons (SPPPs). It is worthwhile noting, that extraordinary modal characteristics are anticipated to emerge because of the large values of $\mathrm{Re}\left(\varepsilon_{LiF}\right)$ at the frequencies below but close f_{TO}. Herein, we deal with the graphene-LiF heterostructure on glass structure. The characteristics of the SPPPs of the waveguide structure at t = 10 nm are presented in Fig. 5. In Fig. 5, one can see that SPPPs dispersion drastically differs in comparison with SPhPs case of the 10 nm-thick LiF waveguide in Fig. 4. It is seen in Fig. 5, that inclusions of the additional graphene layers modifies the dispersion maps, however, the asymptotic frequency and, therefore, the frequency range of propagation of surface waves remains approximately the same for the considered cases (N=1:5). The former approach is needed from the perspectives of the manufacturing techniques. Fabrication of the structure with the thicker layer of graphene sheet requires less technological procedures and efforts. Due to the plasmon-phonon coupling, first, the SPPPs can be supported at significantly smaller wavenumbers. Moreover, backward SPPPs can propagate inside the waveguide for two frequency ranges. The air/graphene/glass and air/LiF/glass waveguide separately can not allow for these two features without combining them in one structure. It is worthwhile noting, that we have obtained results for different number of graphene layers in the compound. It should be mentioned that increase of the number of graphene layers allows to guide the surface waves at lower propagation constants.

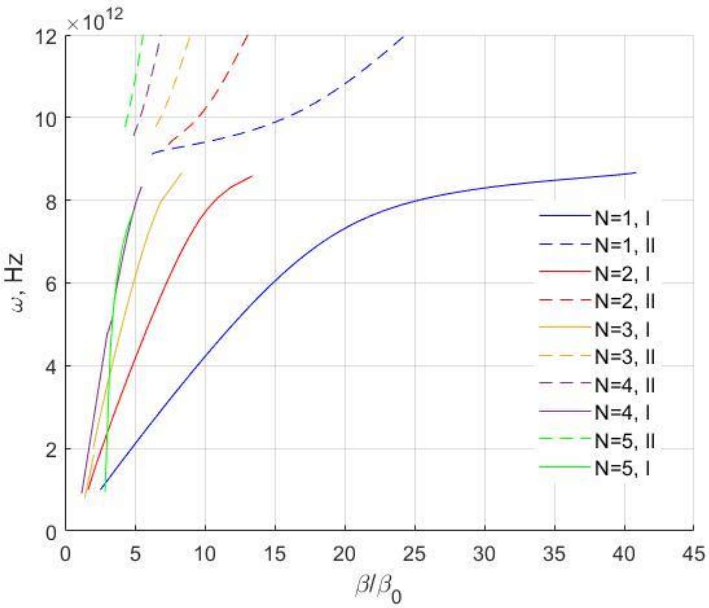


Figure 5. Dispersion of the SPPPS guided by air/graphene/LiF/glass waveguide with t=10 nm. Here, μ=0.2 eV.

Coupling between the highly confined graphene SPPs and the lowly confined SPhPs of air/LiF/glass system for the larger values of the thickness of LiF stands for as a challenging task that is worth to be investigated. The case of t=100 nm is depicted in Fig. 6. As it is demonstrated in Figs. 5-6, modifying number of graphene layers in the structure provides additional degree of freedom aiming to adjust the frequency range of the surface wave existence.

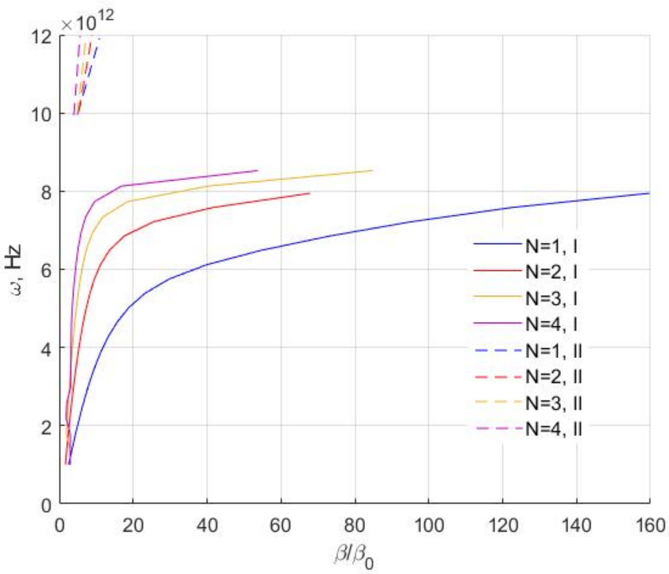


Figure 6. Dispersion of the SPPPs guided by the air/graphene/LiF/glass waveguide for *t*=100 nm.

To have a deeper insight into the physical properties of the SPPPs guided by the structure under consideration in Figs. 5, 6, it is worthwhile noting, that the quasi-bound, leaky part of the dispersion relation is allowed due to the fact, that Re(β)≠0. Thus, β does not tend to infinity as the surface plasmon frequency is approached, but folds back. Moreover, the sketched graphs imply the presence of the surface waves propagating for a long distance. This is caused by the fact that the real part of β is very low within this spectral region.

SPPs of graphene/LiF heterostructures

Aiming to have a further insight into the engineerable properties of SPPs, we have combined both materials, i. e. LiF and graphene in one heterostructure as depicted in Fig. 7.

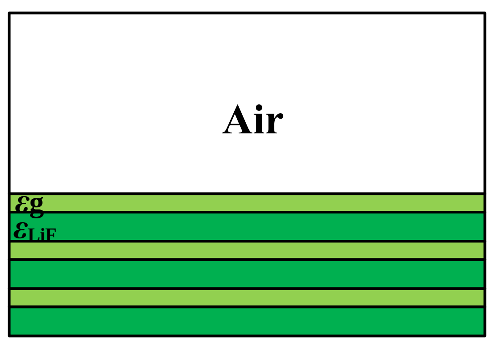


Figure 7. An interface separating infinite layered nanostructured metamaterial formed by alternating graphene and LiF layers and air.

The former approach allows us to benefit from tunability of graphene and wide permittivity range of LiF. The dispersion diagrams of SPPs propagating at the metamaterial interface are presented in Fig. 8.

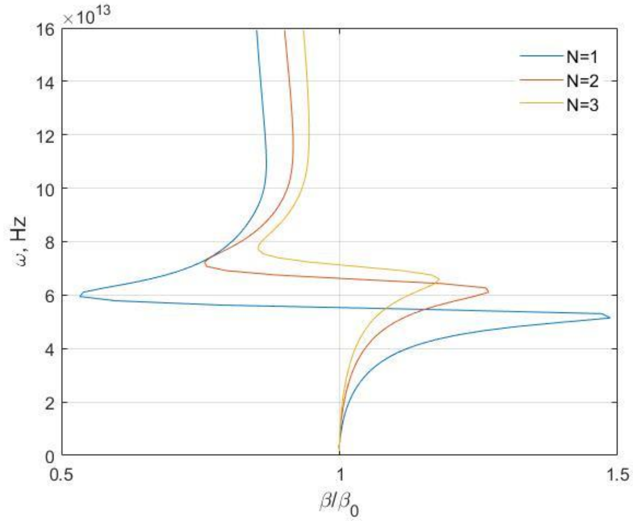


Figure 8. Dispersion supported by graphene/LiF heterostructure.

Comparing Fig. 8 and Fig. 2(b) one may conclude, that enhancement of the dispersion is properties is possible by combining graphene and LiF materials in one single structure. Doing so, one may observe increase of the frequency range of surface waves existence in Fig. 8.

Conclusion

To conclude, two types of the structures with graphene and one auxiliary structure with LiF, a polar dielectric, have been theoretically investigated. Doing so, surface waves in the far-IR region may be supported. Graphene paving the way to support low-loss tunable SPPs in the THz and IR regions has attracted great interest within the scientific community. The former is enhanced by the fact that graphene is one atom thick material. Alternatively, LiF is a strongly dispersive phononic material able to guide SPhPS within the Reststrahlen band (polaritonic gap). Consequently, merging graphene and LiF components in one structure allows for the surface waves with the enhanced and exotic characteristics at the far-IR region allowing to benefit from both, tunability of graphene and a wide permittivity range of LiF. Finally, we investigated the effects possible because of merging graphene with a thin film of LiF and a glass substrate in one structure. Doing so, the effects of wide-range permittivity of LiF and tunability of graphene co-exist. It is worthwhile noting that enhancement of the metamaterial properties is possible by composing it from graphene and LiF building blocks.

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