Propagation of Amplified Surface Plasmon polaritons in AB-stacked Bilayer Graphene

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Abstract
Surface plasmon polaritons (SPPs) are electromagnetic waves that travel along a metal–dielectric or metal–air interface, practically in the infrared or visible-frequency. The term "surface plasmon polariton" explains that the wave involves both charge motion in the metal ("surface plasmon") and electromagnetic waves in the air or dielectric ("polariton") [1]. Due to the short-lived nature of this inverted state, experimental evidence of active plasmons in graphene has so far been elusive. As a result of this ultrashort-lived transient state, a consequence of the absence of an electronic gap, the observation of optical gain (negative conductivity) associated with the inverted state has been elusive in experiments [2]. In this paper the existence of a resonant optical gain at frequencies around the energy gap due to a singularity in its joint optical density of states has been predicted theoretically. Thus, the task is to find the physical and Comsol modelling condition of graphene SPPs simulation with gain. Using the electric conductivity frequency dependence for AB-stacked bilayer graphene with a tunable electronic band gap up to 300 meV data taking from [2], the AB-stacked bilayer graphene thin layer has been designed in 2D Comsol model.
We use Comsol Multiphysics 6.0 Wave optics module to setup AB-stacked bilayer graphene model at THz frequency band. We took a 2D model structure with monolayer graphene layer between air and dielectric substrate as the initial model from Application Libraries site file - graphene_spp.mph. Our studied structure consists of two air layers and a thin AB-stacked bilayer graphene layer between of them.
Using the dependence of real and imaginary part of the electric conductivity of the AB-stacked bilayer graphene presented in [2] we have calculated the dispersion dependences of wave number real and imaginary parts for graphene SPPs. It was obtained two gain regions (44-65 THz, 105-140 THz), where the real conductivity part is negative and the imaginary part of wave number is positive, and SPPs can be expected with gain in graphene. We have estimated SSPs propagation length for the gain regions and have obtained that the propagation length has more than zero absolute values, mainly, in the band of 103-114 THz approximately. Thus, the damping, zero-damping and gain SPPs can be exist in studied graphene only in this band.
The numerical Comsol simulation confirmed that GSPPs with gain were observed using 2D model for the AB-stacked bilayer graphene layer between air areas and there is a quite good agreement with the theoretical data but only for narrow frequency range around 105 THz.
The obtained modelling evidence of the gain SPPs in graphene existence gives the opportunities to greatly increase the SPPs propagation length in graphene layers. It can be used in designing and fabricating nanostructures with desired optical properties.
Keywords: Surface plasmon polaritons, electric conductivity, monolayer graphene, AB-stacked bilayer graphene, dispersion dependences, propagation length.

Introduction

Simulation of surface plasmon-polaritons in monolayer graphene
The science and engineering of subwavelength light-matter interactions have moved to the design and fabrication of nanostructures with desired optical properties. The flexibility associated with the application of such nanostructures as advanced artificial 2D materials (metasurfaces) opens new areas in optics and photonics [1,2]. Surface plasmon polaritons (SPPs) are electromagnetic waves confined to a metal–dielectric interface but free to propagate along it. The term "surface plasmon polariton" explains that the wave involves both charge motion in the metal ("surface plasmon") and electromagnetic waves in the air or dielectric ("polariton") [3]. Graphene surface plasmon polaritons (GSPPs) are characterized by high carrier mobility, strong confinement, low dissipation and high tunability and have been considered for numerous applications including high-density polaritonic circuits, interface with optical data links, photodetectors, surface plasmon waveguides, metamaterials and nanolasers [4].

GSPPs simulation with gain in a 2D model
Graphene has emerged as one of the promising platforms to observe plasmonic effects and light-matter interactions, including the possibility of achieving gain and thus dramatically improved

plasmon-polaritonic coherence without the need for cryogenic temperatures. In [5] the existence of a resonant optical gain at frequencies around the energy gap due to a singularity in its joint optical density of states has been predicted theoretically. In order to facilitate experimental research for GSPPs with reduced dissipation and, potentially, amplification, we carried out Comsol modelling simulations to determine the optimal parameters for their observation. We have carried out such simulations in a 2D model as a first step using the previously determined frequency dependence of the optical conductivity for AB-stacked bilayer graphene presented in [5].

Theory

Optical conductivity of monolayer graphene

To determine the monolayer graphene electric conductivity σ, we use the Kubo formula (Eq.1) [4,6]. The frequency dependence of σ real and imaginary is presented in Fig.1 for the Fermi level is set to 0.2eV.

$$\sigma = \sigma_{intra} + \sigma_{inter}, \qquad (1)$$

$$\sigma_{intra} = \frac{2k_B T e^2}{\pi\hbar} \ln\left(2\cosh\frac{E_F}{2k_B T}\right)\frac{-j}{\omega - j\tau^{-1}},$$

$$\sigma_{inter} = \frac{e^2}{4\hbar}\left[H\left(\frac{\omega}{2}\right) - j\frac{4\omega}{\pi}\int_0^\infty \frac{H(\Omega) - H\left(\frac{\omega}{2}\right)}{\omega^2 - 4\Omega^2}d\Omega\right],$$

$$H(\Omega) = \frac{\sinh\left(\frac{\hbar\Omega}{k_B T}\right)}{\cosh\left(\frac{\hbar\Omega}{k_B T}\right) + \cosh\left(\frac{E_F}{k_B T}\right)},$$

where k_B is Boltzman constant, T is temperature, e is the elemental charge, $\hbar$ is reduced Plank constant, E_F is Fermi energy, $\omega = 2\pi f$, f is operating frequency, τ tau is scattering time.

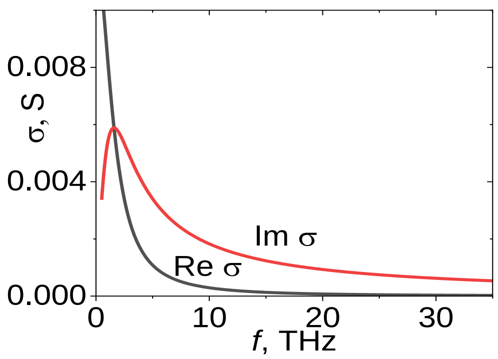

Fig.1. Frequency dependence of the real and imaginary parts of the optical conductivity σ of monolayer graphene.

Dispersion equation of GSPPs

The dispersive equations for monolayer graphene between two dielectrics are as follows [6] for transverse magnetic (*TM*) mode that has *Ex, Ez, Hy* – field components

$$\varepsilon_1 k_2 + \varepsilon_2 k_1 + \frac{i\sigma k_1 k_2}{\omega\varepsilon_0} = 0 \qquad (2)$$

and for transverse electric (*TE*) mode (*Hx, Hz, Ey* – field components)

$$k_1 + k_2 - i\mu_0\sigma\omega = 0, \qquad (3)$$

where $k_m^2 = q^2 - \frac{\omega^2\varepsilon_m}{c^2}$, q - wave number along *x*-axis, where the graphene layer located, *m*=1,2 are dielectric area numbers, ε_m - the permittivity of semi-planes above (*m*=1) and below (*m*=2) the graphene layer.

Simulation Results and Discussion

GSPPs simulation in monolayer graphene layer

Our Comsol 2D model structure consists of a single graphene layer suspended in air. The model has an input wave port 1 on the left edge and an output port 2 on the right edge of the 2D model area shown in Figure 2. As one can see, the amplitude of electric field decreases along *x* direction due to damping in graphene layer.

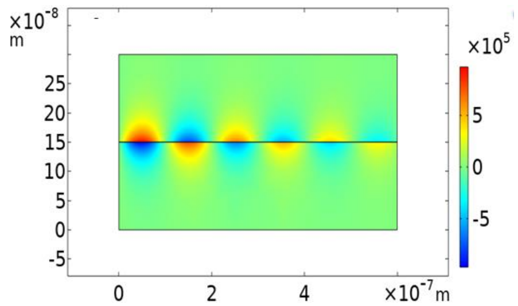

Fig.2. The working area with graphene layer between two semiplanes with the GPPs propagation as the electric E_x- field component distribution along the x-axis at 30 THz for TM mode.

Figures 3 and 4 show the frequency dispersive and dissipative properties of GSPPs and the GPPs propagation length dependence is as follows

$$L = \frac{1}{2\cdot Im(q)}. \qquad (4)$$

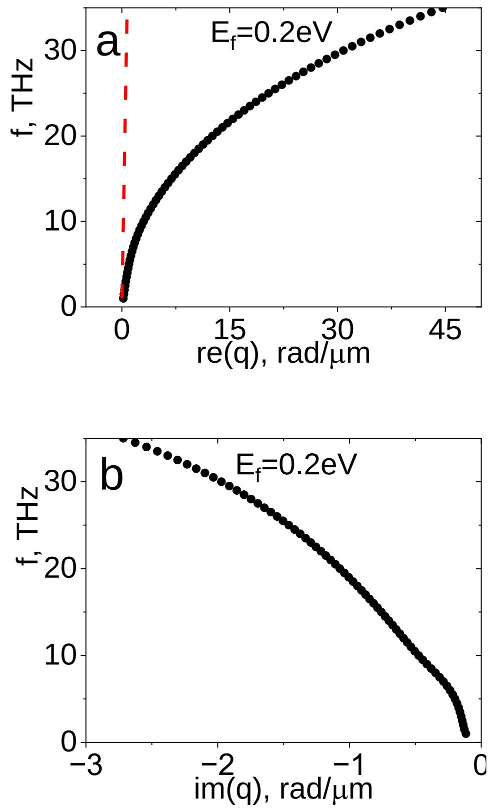

Fig. 3. *The dispersion frequency dependence of the GSPPs, f, on the real (a) and imaginary (b) part of the in-plane wave number q (Eq. 2) along the propagation direction. The photon dispersion (light line) is shown as a red dashed line.*

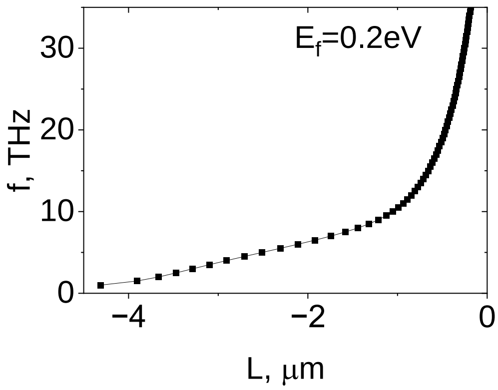

Fig. 4. The frequency dependence of the GPPs propagation length, L.

GSPPs simulation in AB-stacked bilayer graphene

Figure 5 presents the dependence of real and imaginary part of the optical electric conductivity, *σ,* of AB-stacked bilayer graphene presented in [5] for the relevant frequency range. The real part of optical conductivity describes dissipative properties and, therefore, the regions with negative values correspond to energy gain in the GSPPs. There are two such regions in Fig. 5: 44-65 THz and 105-140 THz. We have estimated GSSP propagation length for the gain regions using the relation Eq.4. As shown in Fig.7, the GSSP propagation length *L* in AB-stacked bilayer graphene can be much less than zero (damping state, 104 – 105.1 THz), at definite frequency, approximately at 105.1 THz (see Fig.8) it is zero (zero-damping state), and it is more than zero (gain state, 105.1 -114 THz). In the rest of the region with negative real part of electric conductivity L values are very small (4–20 nm). It means that no GSPPs propagation exists in these frequency ranges.

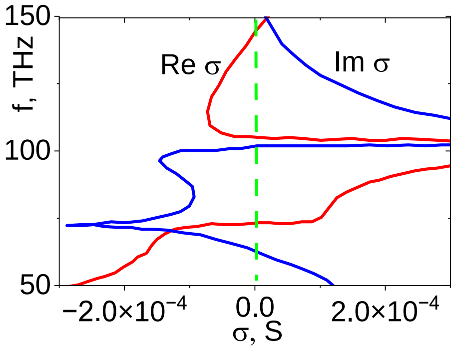

Fig.5. The frequency dependence of the real and imaginary parts of the optical conductivity σ of AB-stacked bilayer graphene [5]. Dashed green line is zero level for of the optical conductivity.

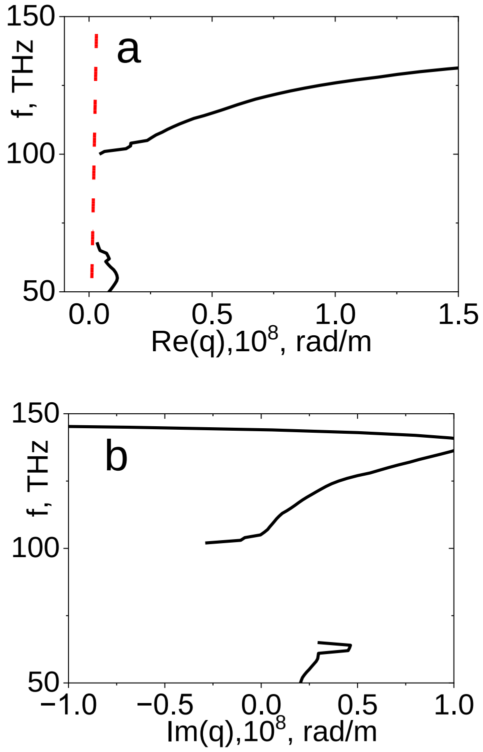

Fig. 6. The dispersion frequency dependence of the GSPPs, f, on the real (a) and imaginary (b) part of the in-plane wave number q along the propagation direction for AB-stacked bilayer graphene. The photon dispersion (light line) is shown as a red dashed line.

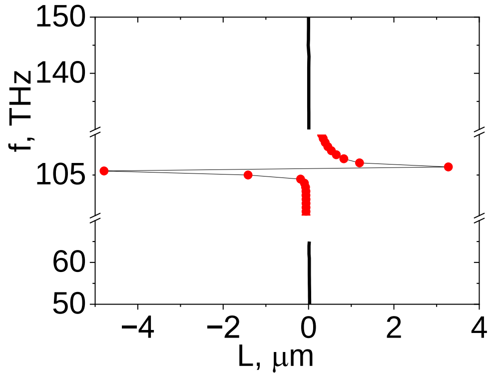

Fig.7. GSPPs frequency dependence on its propagation length L in the bilayer graphene around the gain/loss area with large propagation length shown as red points.

Figure 8 shows the E_x- electric field component distribution along the bilayer graphene layer. Consistent with expectations based on Fig. 7 we observe GSPPs propagation with damping at 104.9 THz (where the real part of the optical conductivity is positive), no damping at 105.1 THz (where the real part of optical conductivity is vanishingly small), and GSPP propagation with gain at 105.9 THz (where the graphene optical conductivity is negative).

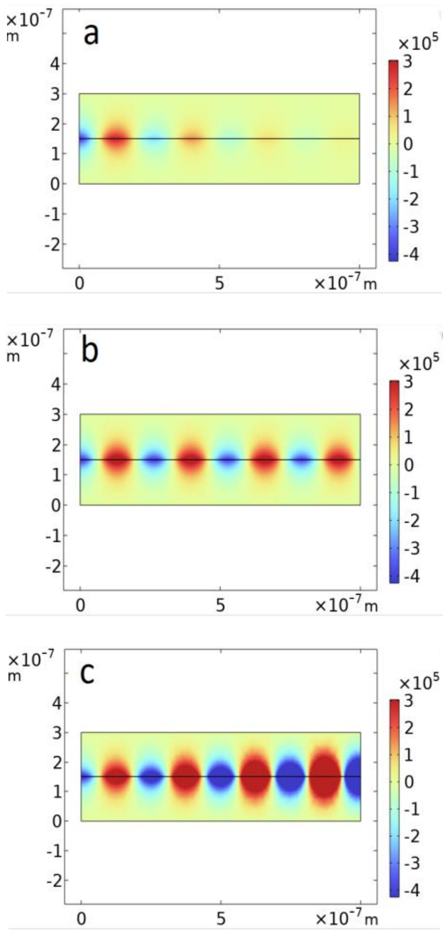

Fig.8. Electric field (E_x-component) distribution along graphene layer in 2D model, (a) – (c) at 104.9, 105.1, and 105.9 THz, respectively.

Conclusions

The numerical Comsol simulation confirmed that GSPPs with gain were observed using 2D model for the AB-stacked bilayer graphene layer between air areas and there is a quite good agreement with the theoretical predicted data.
We have determined that the GSSPs propagation length in AB-stacked bilayer graphene can be much less than zero for the damping state in the range of 104 – 105.1 THz. The GSSPs propagation length is zero for the zero-damping state approximately at 105.1 THz and more than zero for the gain state at 105.1 -114 THz. In the rest of the region with negative real part of electric conductivity L values are very small and no GSPP exists in these frequency ranges.
The obtained modelling evidence of the gain SPPs in AB-stacked bilayer graphene existence gives the opportunities to greatly increase the SPPs propagation length in graphene layers. It can be used in designing and fabricating nanostructures with desired optical properties.

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