Silicon waveguides with graphene: coupling of waveguide mode to surface plasmons

Jiří Čtyroký1, Jiří Petráček2,3, Vladimír Kuzmiak1, Pavel Kwiecien4 and Ivan Richter4

1 Department of Fiber Lasers and Nonlinear Optics, CAS Institute of Photonics and Electronics, Chaberská 57 18251, Prague, Czech Republic
2 Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2 61669, Brno, Czech Republic
3 Central European Institute of Technology, Brno University of Technology, Purkyňova 656/123 61200, Brno, Czech Republic
4 Department of Physical Electronics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Břehová 7 11519, Prague 1, Czech Republic

E-mail: ctyroky@ufe.cz

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Abstract
Silicon waveguides with graphene layers have been recently intensively studied for their potential as fast and low-power electro-optic modulators with small footprints. In this paper we show that in the optical wavelength range of 1.55 µm, surface plasmons supported by the graphene layer with the chemical potential exceeding ~0.5 eV can couple with the guided mode of the silicon waveguide and affect its propagation. On the other hand, this effect might be possibly utilized in technical applications like a very low-power amplitude modulation, temperature sensing, etc.

Keywords: silicon photonics, electrooptic modulation, graphene, surface plasmons

1. Introduction
Two-dimensional (2D) materials, with graphene as their most well-known representative, have been recently successfully implemented into various guided-wave photonic devices, especially modulators, due to their ability to efficiently modify the phase and/or amplitude of propagating guided modes [1–20]. Strong dependence of the surface conductivity of graphene on the chemical potential (or Fermi level energy), controlled by either doping or applied voltage, makes it possible to modify the complex effective refractive index of an optical waveguide with a graphene sheet overlay [21]. For the optical communication wavelength range of 1550 nm, a graphene layer with the chemical potential $\mu_c$ below about 0.5 eV introduces a very strong optical attenuation, while for $\mu_c > 0.5$ eV the attenuation is low while the real part of the effective refractive index is changed. In principle, a graphene layer can thus be utilized for both amplitude and phase electro-optic modulation.

We have recently compared various approaches to numerical modelling of light propagation in a silicon waveguide with graphene overlay [22], and we revealed quite irregular fluctuations of both attenuation and phase of the guided mode in dependence of the chemical potential above approximately 0.5 eV. At first, this effect appeared to be a numerical artifact of the simulation method used, however it was reproduced also in other, completely independent simulation approaches, and it was reported in [23]—see figure 1. Since we were interested in the mechanism behind this effect, we decided to analyze it...
The geometrical parameters of the waveguide structure are close to those used in practical devices: the total silicon layer thickness is $h = 220$ nm, the rib waveguide width is $w = 450$ nm, the residual silicon thickness after the shallow etch is $d = 50$ nm. The graphene layer is deposited only on the top of the rib waveguide, separated from silicon with a thin SiO$_2$ layer, $t = 10$ nm. The superstrate is air. The wavelength of the optical wave propagating in the waveguide is 1550 nm.

The paper is organized as follows: in the next section, we review the properties of surface plasmons at the vacuum optical wavelength of 1550 nm supported by a graphene layer, and present an approximate solution of plasmonic modes propagating along the graphene stripe. Then we describe a simplified coupled-mode theory for the coupling of the multitude of graphene plasmonic modes with the mode of the silicon waveguide and confirm the qualitative CMT results with a ‘rigorous’ full-wave numerical electromagnetic solution obtained with COMSOL Multiphysics [25]. In the final section, we discuss the effect of coupling of the surface plasmons with the waveguide mode on the physical properties of the waveguide structure that may be useful in design and operation of silicon photonic devices with graphene layers.

2. Surface plasmons on graphene

Although the properties of surface plasmons supported by a graphene layer have already been analyzed in detail [24, 26–28], most publications concentrate on the mid-infrared spectral region. We thus first review the properties of surface plasmons at the telecom wavelength band of 1550 nm propagating along the graphene sheet sandwiched between two dielectric media—in this case SiO$_2$ and air. The optical properties of a graphene monolayer are determined by its complex surface conductivity $\sigma_s$, which can be described with an approximate expression [1, 27] (note that we use the convention $\text{exp}(-i\omega t)$ for time-harmonic quantities):

$$\sigma_s(\omega, E_F, \tau, T) \approx \frac{e^2 \mu_e}{\pi \hbar^2} \frac{i}{i/\tau + \omega} + \frac{e^2}{4\hbar} \left[ \frac{1}{2} \left\{ \tan \left( \frac{\hbar \omega + 2\mu_e}{4k_B T} \right) + \tan \left( \frac{\hbar \omega - 2\mu_e}{4k_B T} \right) \right\} - i \frac{\ln \left( \frac{(\hbar \omega + 2\mu_e)^2}{(\hbar \omega - 2\mu_e)^2 + (2k_B T)^2} \right)}{2\pi} \right].$$

(1)

Here, $\omega$, $\mu_e$, $\tau$, $T$, $k_B$ and $\hbar$ are the circular frequency of light, the chemical potential of the graphene layer, the time constant corresponding to the graphene relaxation time, the absolute temperature, the Boltzmann constant and the reduced Planck constant, respectively. We used the following values in our simulations: $\omega = 1.216 \times 10^{15}$ s$^{-1}$ (corresponding to the optical free-space wavelength of 1550 nm), $\tau = 0.2$ ps, and $T = 300$ K. The dependences of the real and imaginary parts of the surface conductivity on the chemical potential, calculated from (1) for $\lambda = 1550$ nm, are shown in figure 2. Note that in the range of $\mu_e > 0.5$ eV, the positive imaginary part of the surface conductivity strongly prevails.

This is a condition allowing propagation of a surface plasmon at the interfaces of a graphene layer, considered as an
ininitely thin layer with a finite surface conductivity \( \sigma_s \), sandwiched between two dielectrics.

### 2.1. Surface plasmon on an infinite graphene sheet

For further considerations, we need to know the surface plasmon propagation constant and field distribution in dependence of the chemical potential of the graphene layer with parameters given above. Let us first consider propagation of a (TM polarized) surface plasmon in the \( z \) direction on a planar structure unlimited in the \( \pm x \) direction (the coordinates axes are considered as in figure 1). Such a wave has a single magnetic field intensity component \( H_y \) and two electric field intensity components \( E_x \) and \( E_z \). Their field distributions in dielectric media are

\[
(H_x, E_y, E_z) = (H_{x,1}, E_{y,1}, E_{z,1}) e^{ik_0 N_{sp} z - k_{sp} y}, \quad y > 0,
\]

\[
(H_x, E_y, E_z) = (H_{x,2}, E_{y,2}, E_{z,2}) e^{ik_0 N_{sp} z + k_{sp} y}, \quad y < 0,
\]

where \( N_{sp} = \beta_{sp}/k_0 \) is the (complex) effective refractive index of the surface plasmon, also called a modal index [29]. \( \beta_{sp} \) is the propagation constant, \( p_1 = (N_{sp}^2 - \varepsilon_{\text{air}})^{1/2} \) and \( p_2 = (N_{sp}^2 - \varepsilon_{\text{SiO}_2})^{1/2} \) are the (normalized complex) transverse decay constants into air and \( \text{SiO}_2 \) substrate, respectively, and \( k_0 = \omega \sqrt{\mu_0 / \varepsilon_0} \) is the vacuum wavenumber.

Next, it follows from Maxwell equations that

\[
E_{x,1} = Z_0 N_{sp} H_{x,1}, \quad E_{x,2} = Z_0 N_{sp} H_{x,2}, \quad Z_0 = \sqrt{\varepsilon_0 / \varepsilon_0},
\]

\[
E_{z,1} = -iZ_0 p_1 H_{x,1}, \quad E_{z,2} = iZ_0 p_2 H_{x,2}.
\]

The field continuity conditions at the graphene layer sound as

\[
E_{z,2} = E_{z,1}, \quad H_{x,2} - H_{x,1} = \sigma_s E_z.
\]

The dispersion equation for the surface plasmon is then obtained from (3) and (4) in the form

\[
\frac{\varepsilon_{\text{air}}}{p_1} + \frac{\varepsilon_{\text{SiO}_2}}{p_2} = -iZ_0 \sigma_s.
\]

Realizing that \( p_2 = (p_1^2 + \varepsilon_{\text{air}} - \varepsilon_{\text{SiO}_2})^{1/2} \), this equation can be cast into the fourth-degree polynomial in the variable \( p_1 \). However, not all roots of this polynomial also satisfy the original dispersion equation (5). Moreover, according to (2), the existence of the surface plasmon as a physically realizable wave confined to the graphene layer and decaying in the direction of propagation requires that the real parts of both \( p_1 \) and \( p_2 \) and the imaginary part of the effective refractive index \( N_{sp} = (p_1^2 + \varepsilon_{\text{air}})^{1/2} \) are positive. At the wavelength of 1550 nm, just one surface plasmon wave is supported in our structure in the range of the chemical potential \( \mu_s \), considered in figures 3 and 4. These figures show real and imaginary parts of the effective refractive index of the surface plasmon, its propagation length \( L_{sp} = 1/[2k_0 \text{Im}(N_{sp})] \), and its penetration depths into air and \( \text{SiO}_2 \), \( d_{air} = 1/(k_0 \text{Re}(p_1)) \) and \( d_{\text{SiO}_2} = 1/(k_0 \text{Re}(p_2)) \), respectively.

Note that in the range of \( \mu_s > 1 \text{ eV} \), the propagation length typically reaches a fraction of a micrometer, and the penetration depths into both dielectric media are practically the same, of the order of a few nanometers, due to the very large effective index of the plasmon mode, \( p_1 \approx p_2 \approx N_{sp} \). From this approximation and (3), it also follows that electric field intensity components are practically equal in magnitude, although mismatched in phase, \( E_z \approx -iE_{x,1} \approx iE_{x,2} \), and magnetic field components are scaled with respect to the permittivities of the surrounding media, \( H_{x,1}/\varepsilon_{\text{air}} \approx -H_{x,2}/\varepsilon_{\text{SiO}_2} \). A very strong vertical confinement of the surface plasmon justifies the fact that the proximity of silicon was neglected in this analysis. Its influence will be taken into account later in the CMT approach.
2.2. Surface plasmons on a graphene stripe

The surface plasmon mode propagating in the z direction, described in the previous section, cannot couple with the guided mode of the silicon waveguide because of a huge (1–2 orders of magnitude) mismatch of their effective refractive indices (note that the effective refractive index of the quasi-TE mode of the silicon waveguide at $\lambda = 1550$ nm calculated with COMSOL is 2.3754). However, the graphene stripe on top of the silicon ridge waveguide in figure 1 supports a number of higher order (‘nanoribbon’ [24, 30–32]) modes with smaller propagation constants, and some of them can match with that of the mode of the silicon waveguide. We will use the approach of the effective-index method (EIM) [33] to approximately determine their propagation constants and field distributions. Similarly to a mode of a planar dielectric waveguide, the plasmonic modes of a graphene stripe result from the interference of two plasmons that are propagating under some angle with respect to the z axis and are reflecting from the stripe edges. Following the idea of the EIM, the dispersion equation for such modes can be written in the form of the transverse resonance condition (in the x direction)

$$R^2 \exp(2ik_0wq_m) = 1,$$

where $k_0wq_m$ is the transverse propagation constant of the $m$th mode, $m$ is the mode number, and $R$ is the (amplitude) reflection coefficient of the plasmon from the edge of the graphene stripe.

Reflection and scattering of a surface plasmon from discontinuities in the graphene plane—including the reflection from the edge of a graphene stripe—has already been studied in detail and reported in a number of recent papers [31, 34–39]. It has been found that the reflection at the stripe edge is close to the total, $|R| \approx 1$, while the phase of the reflection coefficient non-trivially depends on the detailed morphology of the graphene edge, on the inhomogeneity of the graphene conductivity due to redistribution of charges, on the excitation of evanescent waves near the stripe edge, etc. To keep our analysis as simple as possible, we decided not to consider this anomalous phase shift. Numerical tests with various kinds of boundary conditions (perfectly electric or magnetic (PMC) walls and Fresnel reflection coefficients) finally led us to the application of the PMC approach. This choice allows for a very simple evaluation of the effective refractive indices and the electromagnetic field distributions of the graphene stripe modes, which are quite close to those obtained by using more rigorous COMSOL simulations. Some lowest-order modes of the graphene stripe (including central and edge ‘ribbon plasmons’ [32]) are out of scope of this approach. However, these modes cannot couple with the mode of a silicon waveguide due to strong mismatch of their propagation constants.

By taking $R^2 = 1$, we obtain the solution of the dispersion equation (6) in the form

$$q_m = \frac{m\pi}{k_0W}, \ m = 1, 2, \ldots$$

$$N_m = \sqrt{N_{sp}^2 - q_m^2},$$

where $q_m$ are real numbers. Since $N_{sp}$ is complex, the effective refractive indices $N_m$ are complex too. Consequently, there is no clear transition between propagating and evanescent plasmonic modes of the graphene stripe. However, since the imaginary part of $N_{sp}$ is significantly smaller than its real part, the real parts of high-order modes $N_m$ reach low enough values for efficient coupling with the fundamental (quasi-)TE silicon waveguide mode. However, their imaginary parts are nonzero, which indicates that the coupling may introduce a rather significant loss. As an example, the real and imaginary parts of the effective refractive indices $N_m$ of the graphene stripe are plotted in figure 5 for two values of the chemical potential, $\mu_c = 1.0$ and 1.61 eV.

In our approximation, $q_m$ are real numbers. Since $N_{sp}$ is complex, the effective refractive indices $N_m$ are complex too. Consequently, there is no clear transition between propagating and evanescent plasmonic modes of the graphene stripe. However, since the imaginary part of $N_{sp}$ is significantly smaller than its real part, the real parts of high-order modes $N_m$ reach low enough values for efficient coupling with the fundamental (quasi-)TE silicon waveguide mode. However, their imaginary parts are nonzero, which indicates that the coupling may introduce a rather significant loss. As an example, the real and imaginary parts of the effective refractive indices $N_m$ of the graphene stripe are plotted in figure 5 for two values of the chemical potential, $\mu_c = 1.0$ and 1.6 eV.

A full-vector field distribution of plasmon stripe modes is given by the superposition of two surface plasmons with equal amplitudes and with the wave vectors $k_{m1} = k_0 (\pm q_m, i\pi_1, N_m)$, $k_{m2} = k_0 (\pm q_m, -i\pi_2, N_m)$, where the sign $\pm$ relates to the direction of propagation in the $(x, z)$ plane, and the subscripts 1, 2 are related to the regions $y > 0$ and $y < 0$, respectively, in accordance with (2). Note that all components of electric and magnetic fields are nonzero, except for $H_y$.

Basics of the CMT describing simultaneous coupling of the mode of the silicon waveguide with several plasmon modes of the graphene stripe are briefly described in the next session.

3. Coupling of waveguide mode with surface plasmons on graphene stripe

Simultaneous coupling of a mode of a silicon waveguide with several plasmonic modes of a graphene stripe on top of the silicon waveguide can be considered as mutual coupling.
among modes of several parallel waveguides. One of the waveguides is the silicon waveguide, while the other ‘waveguides’ correspond to individual plasmonic modes supported by the graphene stripe. We denote the field distribution of the eigenmode of the silicon waveguide without graphene as

\[ E_1 = e_1(x,y) \exp(i\beta_1 z), \quad H_1 = h_1(x,y) \exp(i\beta_1 z), \]  

(9)

where \( \beta_1 \) is its propagation constant. Similarly, the field distributions of plasmonic modes are

\[ E_m = e_m(x,y) \exp(i\beta_m z), \quad H_m = h_m(x,y) \exp(i\beta_m z), \]  

(10)

where \( M \) is the number of plasmonic modes taken into account.

In this approach, the eigenmodes (‘supermodes’) of the complete waveguide system with the (generally complex and anisotropic) permittivity distribution \( \varepsilon(x,y) \) are constructed as linear superpositions of eigenmodes of individual waveguides with the corresponding permittivity distributions \( \varepsilon_m(x,y) \),

\[ E_s = e^{\gamma_s} \sum_{m=1}^{M+1} a_{sm} e_m(x,y), \quad H_s = e^{\gamma_s} \sum_{m=1}^{M+1} a_{sm} h_m(x,y), \]  

(11)

where \( \gamma_n \) are the propagation constants and \( a_{sm} \) are the expansion coefficients of the ‘supermodes’. Specifically, \( \bar{\varepsilon} \) is the complete permittivity distribution of the waveguide structure including graphene layer as shown in figure 1, \( \varepsilon_s \) is the permittivity distribution of the silicon waveguide in figure 1 without the graphene layer, and \( \varepsilon_m, m = 2, \ldots, M + 1 \) are identical permittivity distributions containing the graphene stripe on the SiO\(_2\) pedestal of the width \( w \), surrounded by air. Applying the principles of the complex CMT \([40, 41]\) (chapter 10), we arrive to the following generalized eigenvalue equation for the complex amplitudes \( a_{sm} \) and the propagation constants \( \gamma_s \):

\[ \sum_{n=1}^{M+1} \left( \beta_m A_{mn} + \omega \varepsilon_0 C_{mn} \right) a_{mn} = \gamma_s \sum_{n=1}^{M+1} A_{mn} a_{mn}, \]  

(12)

where

\[ A_{mn} = \int_S (e_m \times h_n + e_n \times h_m) \cdot \hat{z} \, dx \, dy, \]

\[ C_{mn} = \int_S e_n \cdot (\hat{\varepsilon}_n - \varepsilon_s) \cdot e_m^\ast \, dx \, dy, \]  

(13)

\[ m, n = 1, 2, \ldots, M + 1. \]

Here, \( e_m^\ast \) denotes the electric field distribution of the \( m \)th mode with inverted \( z \)-component, and \( S \) is the cross-section of the whole waveguide structure. Using similar arguments as in \([22]\), we obtain

\[ C_{tn} = i \alpha_s \int_{-w/2}^{w/2} \left[ e_{1x} e_{tnx} - e_{1z} e_{tnz} \right] yz \, dx, \]  

(14)

\[
\text{Figure 6. The variance of (a) real and (b) imaginary parts of the effective refractive index of the TE mode of the silicon rib waveguide due to graphene stripe as a function of the graphene chemical potential. Blue line: numerical solution using COMSOL, red line: perturbation method (PT), yellow line: coupled mode theory (CMT). Interval of } \mu_c \text{ from 1.4 to 2 eV in figure 6(a) is zoomed in the inset for better resolution.}
\]
of the order of several dB/mm. Figure 7 shows the distribution of the horizontal electric field intensity component of the fundamental TE mode of the silicon rib waveguide coupled with a surface plasmon on the graphene stripe, calculated with COMSOL, for the resonance value of $\mu_c = 1.61$ eV (see figure 6). The ‘decoration’ of the mode field with the field distribution of the surface plasmon is apparent. Note that, according to (13), only surface plasmon modes with the same symmetry can couple with the silicon waveguide mode.

Although the dominant electric field component of the plasmons is vertical ($E_z$), there is curiously negligible coupling among the graphene plasmons and the TM-polarized waveguide mode. The reason stems from the nature of the coupling mechanism. According to (13), only electric field components parallel with the graphene layer can contribute to the coupling; apparently, there is no graphene conductivity in the vertical direction. When a graphene layer is also deposited on the side walls of the silicon waveguide (as was considered, e.g. in [22]), graphene stripe plasmon modes supported by the side walls can contribute to the coupling too. As a result, the (quasi-)TM waveguide mode is also affected, the graphene mode spectrum is more complicated, and so are the phase and attenuation dependences of the waveguide mode on the chemical potential of the graphene layer.

4. Conclusions

Propagation of surface plasmons on graphene sheets has been previously studied, mostly in the THz and infrared frequency ranges. On the other hand, graphene layers on silicon waveguides have recently been used very often in the design and construction of photonic devices for modulation, switching, etc. These devices typically operate within the telecommunication band around 1550 nm, where the surface plasmon propagation on graphene layers has attracted much less attention. In this communication, we show that in the range of the chemical potential of graphene above 0.5 eV, surface plasmons supported by graphene stripes deposited on the top of a silicon waveguides rather strongly affect their guiding properties due to the coupling of surface plasmons with the mode propagating in the waveguide. This effect has been independently studied by both the approximate method based on the CMT, and by ‘rigorous’ numerical simulations using COMSOL. Although the accuracy of the approximate method is not high, it offers a deep insight into the process and contributes to the understanding of the details of the coupling mechanism. The effect has not necessarily been considered harmful for the operation of silicon photonic devices, rather it may be employed in design of specific devices such as low-power modulators and sensors. Although our analysis was focused at the near infrared telecom wavelength range, we are highly convinced that this effect takes place not only in the near- to mid-IR silicon transparency window, but also in the THz spectral range where the silicon waveguides are being used as well [18, 42–44].
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ORCID iD

Jiří Čtyroky © https://orcid.org/0000-0002-4483-1311

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