Mathematical Modelling of Electrically Controlled Filters of Microwave, subTHz and THz–bands on the Base of Graphene-and-Dielectric Multilayer Structure

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Abstract. Report is devoted to investigations of graphene meta–surfaces for the transmission of radiation induced by plasmons in subTHz and THz ranges, cell of which consists of structures based on graphene ring and graphene nano–tape. It create regimes of radiation transmission – transparency windows induced by electric dipole resonances. Resonant frequency of transparency window can be dynamically tuned in wide band of subTHz and THz bands by changing the chemical potential (Fermi energy) of graphene by applying external electric field (gating) instead of re–fabricating of structures. Questions of possibilities of electronic controlled filters creating of subTHz and THz bands grounded on different configurations of graphene meta–surfaces are discussed; their characteristics and frequency dependencies are investigated. Mathematical modelling and electrodynamic calculation of the filters characteristics of subTHz and THz bands grounded on multilayer structures of “graphene–dielectric” type are carried out. From results of mathematical modelling it follows that periodic layered microstructures “graphene–dielectric” type can be used for creation of subTHz and THz bands broadband filters of planar construction, controlling by electric field and fast tuning at small changes in Fermi energy level of graphene.

1. Introduction

Greater agility of the carriers of charge in graphene creates it very prospective substance for application in the diverse equipment as new elemental base for nanoelectronics and feasible substitution of silicon in the integral circuits (chips) and entail making of radioelectronic equipment of microwave, subTHz and THz frequency ranges [1–3].

In [4], graphene meta–surfaces for transmission of radiation induced by plasmons in subTHz and THz range, whose cell consists of the structure based on graphene ring and graphene nano–tape, were investigated. Both graphene rings and graphene nano–tapes create radiation transmission regimes (modes) – the transparency spectral windows induced by electric dipole resonances. The weak hybridization (with weak interaction) between two cells (elements) causes the appearance of new
spectral transparency window induced by plasmons, which can be managed by changing of geometric sizes (dimensions) of based on the graphene meta–surface elementary cell structure [5].

Resonant frequency of the window of spectral transparency can be tuned dynamically in a wide band of subTHz and THz frequencies, changing the value of chemical potential (Fermi energy) of graphene by external electric field application—electrostatic gating instead of re–producing of the structures [6].

2. Purpose of Investigation
The aim of author’s research is making the high–speed controlled filters based on graphene structure in order to develop highly efficient tunable nanophotonic arrangement for signal processing using new principles and modern materials, substances and nanostructures. The objectives of study are to review existing research in the field of graphene and select the most prospective of them. At the following stage, the mathematical modelling of electrically controlled filters of microwave, subTHz and THz ranges based on multilayer “graphene–and–dielectric” nanostructures was carried out. The scientific novelty of the research lies in the implementation of computer simulation of electrodynamics of periodic multilayer nanostructures of “graphene–and–dielectric” type, and the identification of the possibility of using these nanostructures to create broadband filters of microwave, subTHz and THz bands of planar design, controlled by electric field and quickly tunable with little changes in graphene Fermi energy level.

3. Electronically Controlled subTHz / THz Band Filters on Graphene Meta–surfaces
Figure 1 shows the structures of graphene–based meta–surface cells for demonstration the phenomena of radiation induced by plasmons. The basic elemental cell of meta–surface [7] contains graphene ring and graphene nano–tape. Internal and external radiuses of this ring are \( r_1 = 2.0 \mu m \), and \( r_2 = 3.2 \mu m \). The length on nano–tape is \( L = 9.0 \mu m \), and its width \( W = 0.7 \mu m \). Dielectric substrate constitute photopolymer with relative dielectric permeability \( \varepsilon = 2.4 \mu m \) and thickness \( h = 0.5 \mu m \). This structure is located along the directions of \( x \) and \( y \), with the value of period \( p = 10.0 \mu m \). The incident wave falls perpendicularly to the plane “\( x – y \)”, with polarization value \( E_x \).

![Figure 1. Meta–surfaces cells of different configurations: graphene ring operating in the regime of window spectral transparency for the radiation, induced by plasmons.](image)

To demonstrate the effect of radiation induced by plasmons, the frequency dependences of transmission coefficient of passing through the filters based on graphene meta–surface with the elementary cell were calculated. This is composite structure based on graphene ring and graphene nano–tape (curve 3 in the figure 2); single graphene nano–tape (curve 2); and single graphene ring (curve 1); for the value of the chemical potential (Fermi energy) \( \mu_c = 0.5 \text{ eV} \).

From figure 2 it is obviously, that when at unification of graphene ring and graphene nano–tape to some composite structure, oriented along of the direction of electrical field, the window of spectral transparency for subTHz and THz band radiation, induced by plasmons, with transmission coefficient more than 95% is observed at frequencies \( f_1 = 1.68 \text{ THz} \) and \( f_2 = 2.14 \text{ THz} \).
For demonstration of the physical mechanism of plasmon–induced radiation effect, the calculated distribution of electric field for three resonant frequencies of the filter $f_1 = 1.68$ THz, $f_2 = 1.86$ THz, $f_3 = 2.14$ THz is shown as example, which correspond to minimum of transmission coefficient (figure 2).

For the modelling (simulation) of structures based on graphene used computational methods: modified—finite element method (FEM), finite differences methods in the domain time (FTDT), periodic method of moments (MoM), on the ground of which the algorithms are implemented in the well–known commercially available application packages: High Frequency Structure Simulator (HFSS, Ansoft), Advanced Design System (ADS, Agilent), MacNeil–Schwendler (MSC), Microwave Office, Microwave Studio, FEKO, LabVIEW. Authors had opportunity to use the packages ADS, Microwave Office and Microwave Studio.

![Figure 2](image_url)

Figure 2. Frequency dependence of transmission coefficient through the filters based on graphene meta–surfaces for various configurations of meta–surface elements. Curves: 1) Graphene ring; 2) Graphene nano–tape; 3) Structure based on graphene ring and graphene nano–tape.

Result was obtained by authors in the package ADS, Agilent.

In the figure 3 (a) at the first resonance, in the frequency $f_1 = 1.68$ THz, it is seen that nano–tape is excited strongly by existing electric field, and ring is actuated enough feebly. At the second resonance at the frequency $f_2 = 2.14$ THz, shown in the figure 3 (c), the optical response of the ring and nano–tape is mainly concentrated on the ring, which behaves as antenna of optical type, and oscillates with external electric field. Both resonances creates the windows of spectral transparency for THz radiation induced by electric dipole oscillations. Figure 10 (b) demonstrate electric field at the third resonant frequency of $f_3=1.86$ THz. Oscillation of quadrupole type arise in the ring and in the nano–tape, and phase resonance emerge in two composite parts: on the graphene ring and on the graphene nano–tape ones.

Influence of geometric dimensions on the response of THz radiation, induced by plasmons, was investigated numerically. Result is the fact, that with increasing length $L$ of nano–tape, the first resonance $f_1=1.68$ THz is rapidly changing towards lower THz frequencies. The second resonance $f_2 = 2.14$ THz does not change; thus, the interval between two resonances and maxima of transmission coefficient increases. The dependence of resonance frequency on graphene nano–tape length $L$ is plotted. At the length $L$ increasing, the frequency shift (displacement) by second resonance saves its invariance, and the frequency $f_1$ of the first resonance changes very quickly. Similarly, at increasing the width $W$ of the graphene nano–tape, the first resonance is displaced towards higher THz frequencies, while the second resonance saves invariance, and windows of spectral transparency for THz radiation, induced by plasmons, is narrowed sharply.
Figure 3. Electric field distribution for frequencies: a) $f_1 = 1.68$ THz – first minimum of transmission coefficient; b) $f_2 = 1.86$ THz – second minimum of transmission coefficient; c) $f_3 = 2.14$ THz – window of spectral transparency of radiation. Result was obtained by authors in Microwave Studio package and was confirmed in Microwave Office and LabVIEW packages.

Graphene surface conductivity can be varied by managing of its chemical potential (energy of Fermi) $\mu_c$. Chemical doping (alloying) change or electrostatic gating can implement such control. Dynamic control of the windows spectral transparency of the meta-surface is realized without geometry reconstruction or introduction of other controlled materials by varying the chemical potential [8].

In the figure 4, frequency dependences of transmission coefficient at the different values of graphene $\mu_c$ are shown. The window of spectral transparency can be reconfigured (tuned) effortlessly in the wide band of frequencies by small changing of chemical potential $\mu_c$ (energy of Fermi). When $\mu_c$ is increasing from 0.3 to 0.7 eV, the resonance frequencies rise too, from 1.47 to 2.25 THz, thanks to what the window of spectral transparency tunes completely.

Figure 4. Frequency dependencies of transmission coefficient through the filter at the different magnitude of graphene chemical potential. Curves: 1) $\mu_c = 0.3$ eV; 2) $\mu_c = 0.5$ eV; 3) $\mu_c = 0.7$ eV. Result was obtained by authors in the package ADS, Agilent.

4. Computational Algorithm for Calculation of Conductivity and Scattering Matrixes
Mathematical model of electromagnetic waves diffraction is developed; their interactions with multilayer micro- and nanostructures of “graphene–and–dielectric” type based on the solution of diffraction problems for Maxwell’s equations in conjunction with material equation of graphene medium, where the surface conduction of graphene is included as parameter, and the electrodynamical boundary conditions are investigated. Graphene monolayer is characterized by surface conductivity that is determining by Kubo formula [9]:
\[
\sigma(\omega, \mu) = -ie^2 k_i T \left( \frac{\mu_e}{k_i T} + 2 \ln \left( \exp \left( -\frac{\mu_e}{k_i T} \right) + 1 \right) \right) - \frac{ie^2(\omega - i2\Gamma)^4}{\pi \hbar^2} \int_0^\infty \left( \exp \left( -\frac{\xi - \mu}{k_i T} \right) + 1 \right)^{-1} - \left( \exp \left( \frac{2\xi}{\hbar} \right) \right)^{-1} d\xi.
\]

(1)

where \( e = 1.6 \cdot 10^{-19} \) C – the electron charge; \( k_b = 1.38 \cdot 10^{-23} \) J/K – the Boltzmann constant; \( h = 1.054 \cdot 10^{-34} \) J/s – the Planck constant; \( T = 300 \) K – the temperature; \( \Gamma = 10^{12} \) 1/s – the relaxation speed; \( \mu_e = 0 - 1 \) eV – the chemical potential (1 eV=1.602·10^{-19} J); \( \omega = 2\pi f \) – the frequency.

The filter of THz band is considered as waveguide transformer with Floquet’s channels, between the input cross–sections \( S_1 \), \( S_2 \) of which the multilayer structure of type “graphene–and–dielectric” is situated. As waveguide transformer descriptor the scattering matrix \( S \) is used. The multilayer structure of type “graphene–and–dielectric” can be considered as cascading FAB connection (Floquet’s Autonomous Blocks) in the form of Floquet’s channels with uniform filling of graphene or dielectric.

Let us determine the matrix \( Y \) of conductivity FAB as segments of Floquet’s channels with uniform filling of graphene (or dielectric) with dielectric and magnetic permeabilities \( \varepsilon \), \( \mu \) and \( \varepsilon^0 \), \( \mu^0 \). The calculated electrodynamic scheme is shown in the figure 5.

**Figure 5.** Floquet’s Autonomous Blocks (FAB) as segments of Floquet channels with uniform filling of graphene (or dielectric) with dielectric and magnetic permeabilities \( \varepsilon \), \( \mu \) and \( \varepsilon^0 \), \( \mu^0 \).

Electromagnetic field in the cavity \( V \) of Floquet’s Autonomous Blocks was found in the form of superposition of direct (forward) and return (backward) waves of Floquet’s channel, homogeneously filled by medium with dielectric and magnetic permeabilities \( \varepsilon^0 \) and \( \mu^0 \): \n
\[
\begin{align*}
\vec{E}^0 &= A_k^0 \left( \vec{e}^{00} + \vec{e}^{01} \right) \exp(-i\Gamma^0 z_1) + A_k^1 \left( \vec{e}^{01} - \vec{e}^{00} \right) \exp(i\Gamma^0 z_1) \\
\vec{H}^0 &= A_k^0 \left( \vec{h}^{00} + \vec{h}^{01} \right) \exp(-i\Gamma^0 z_1) + A_k^1 \left( \vec{h}^{01} - \vec{h}^{00} \right) \exp(i\Gamma^0 z_1)
\end{align*}
\]

(2)

After tedious calculations was found the expression for the matrix \( Y \) of conductivity FAB in the form of segments of the Floquet’s channels with uniform filling by the graphene (or dielectric) with dielectric and magnetic permeabilities \( \varepsilon \), \( \mu \) and \( \varepsilon^0 \), \( \mu^0 \) (figure 5). Elements of the matrix \( Y \) of conductivity Floquet’s Autonomous Blocks are defined as follows [10]:

\[
\begin{align*}
Y_{kn}^{11} &= Y_{kn}^{22} = -i\delta_{kn} \frac{W_k}{\cos \Gamma^0_k} \\
Y_{kn}^{12} &= Y_{kn}^{21} = i\delta_{kn} \frac{1}{\sin \Gamma^0_k} \\
\end{align*}
\]

(3)

Scattering matrix \( S \) is determined from the matrix of \( Y \) of conductivity FAB as:

\[
S = (I + Y)^{-1}(I - Y)
\]

(4)

Multichannel multimode conductivity matrix \( Y \) obtained by combining objects A, B defined as:
\[
Y = Y^{\alpha\alpha} + (Y^{\alpha\beta} + Y^{\alpha\gamma})(Y^{\beta\beta} - Y^{\gamma\gamma})^{-1}(Y^{\gamma\alpha} - Y^{\beta\alpha})
\]

where combinations \(\alpha\alpha, \alpha\beta, \alpha\gamma, \beta\beta, \gamma\gamma, \gamma\alpha, \beta\alpha\) – belongs to the virtual channels.

By connecting all Floquet’s Autonomous Blocks, the conductivity matrix \(Y\) of the filter of THz band, grounded on multilayer structure of “graphene–and–dielectric” type was obtained.

Then the conductivity matrix \(Y\) is recalculated into the scattering matrix \(S\).

5. Electrodynamic Calculation of THz Band Filters Characteristics Based on Multilayer Structure of Type “Graphene –and–Dielectric”

Principles of construction of THz–band filters, controlled by the electric field, are investigated, and the electrodynamic calculation of their characteristics is carried out by the FAB method [11].

The calculation model of subTHz / THz range planar filter grounded on periodical multi–layer structure of “graphene–and–dielectric” type is demonstrated in the figure 6. Algorithm of calculation grounded on FAB method was applied for electrodynamic calculation of elements scattering matrix subTHz/THz filters, based on periodical multi–layer structures of "graphene–and–dielectric" type.

![Figure 6. Calculation model of the planar filter of THz band grounded on periodic multi–layer structure of “graphene–and–dielectric” type.](image)

In the figure 7 are shown the calculated frequency characteristics – dependences of the element \(|S_{21}|\) scattering matrix – transmission coefficient of \(TEM\)–wave (Transverse Electromagnetic wave) through the THz range filter based on multilayer structure "graphene–and–dielectric" with different number \(N\) of graphene sheets \((N = 33, 47, 60)\) for the values of chemical potential \(\mu_c = 0\) eV; \(\mu_c = 1\) eV.

![Figure 7. Frequency dependence of element \( |S_{21}| \), dB, of the filters scattering matrix based on multilayer structures of “graphene–and–dielectric” type with different number of graphene sheets \((N = 33, 47, 60)\) for values of chemical potential \(\mu_c = 0\) eV; and \(\mu_c = 1\) eV: \(h=3.65\) µm; \(\varepsilon_d=2.2\). Result was obtained by authors in the package ADS, Agilent.](image)
From the results of the electrodynamic calculation (figure 7) it follows that with increase of graphene sheets number \((N = 33, 47, 60)\), the transmission coefficient \(\text{S}_{21}\) in the non–transmission band decreases significantly. As the modelling results demonstrate, by changing the chemical potential \(\mu_e\) by the application of external electric field (which leads to change of graphene conductance), it is possible to control the characteristics of filters based on multilayer structures of type “graphene–and–dielectric”.

So, at chemical potential value \(\mu_e = 0\) V (if external electric field absents), THz radiation attenuation in the non–transmission band is \(2–4.5\) dB (depending on the number \(N = 33–60\), respectively). At application of external electric field, which corresponds to chemical potential \(\mu_e = 1\) eV, the attenuation of radiation increases to \(20 – 40\) dB (with change in the number \(N = 33–60\)).

Thus, from the results of modelling it follows that the investigated periodic layered microstructure of type “graphene–and–dielectric” can be used to create the broadband filters of subTHz and THz band of planar construction, controlled by electric field and quickly tunable with small changes of the level of graphene Fermi energy.

6. Conclusion

Investigations fulfilled by authors was purposed at the research of the opportunity for the making of new generation filters of SHF, EHF and HHF (subTHz and THz) bands using new principles, materials and nanostructures. In the scientific primary sources studied by authors, much attention is paid to graphene and based on it nanostructured meta–materials and meta–surfaces.

It was compared with the results of other authors who conducted studies of multilayer structures of the graphene–and–dielectric type. Verification of the results with experimental and simulation results of other authors show the significant coincidence of the constructed graphical dependencies with the results published in the works \([12]\) by R.D. Innocenti and etc., and \([13]\) by J. Wang end etc.

Mathematical model of the filter based on the multilayer structure of type “graphene–and–dielectric” is constructed. It is shown that such filter has stability and resistance in relation to the spread of the values of the surface conductance of graphene sheets included in the investigated filter.

Computational Algorithm for Calculation of Conductivity and Scattering Matrixes was received.

Creation of high–speed controlled filters on graphene ground can develop highly efficient tunable nanophotonic devices for signal processing. The fact was detected that these nanostructures can be applied to create the wideband filters of microwave, subTHz and THz ranges of planar design, controlled by electric field and fast tunable with small changes in Fermi’s energy level of graphene.

Filters based on multilayer structures of type “graphene–and–dielectric” are controlled by changing the chemical potential by displacement of electrical field. At the lack of electrical field, the filter transmits the corresponding radiation, at existence of electrical field – the attenuation of microwave, subTHz or THz radiation can reach \(-40\) dB and above, depending on the number of graphene layers.

The researched structures can be apply for creating of controlled wideband filters of microwave, subTHz and THz ranges of frequency of planar design and construction. Rejection filters built on the base of multilayer structures of “graphene–and–dielectric” type are particularly promising.

As modelling results demonstrate, the change of chemical potential by means of external electric field leads to the modification of graphene conductivity. It is possible to control the transmission coefficient of radiation of corresponding range through filters based on multilayer structures of “graphene–and–dielectric” type \([14] – [17]\).

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