Diffraction by double layer graphene strip grating

Mstyslav E. Kaliberda*, and Sergey A. Pogarsky
V.N.Karazin National University of Kharkiv, Ukraine

Abstract

Diffraction of the *H*-polarized wave by double layer grating of finite number of graphene strips in the THz range is considered. Integral equations relatively unknown spectral function of the scattered field are reduced to the system of singular integral equations. The numerical solution is obtained by the Nystrom-type method of discrete singularities. The scattering and absorption characteristics are represented.

1. Introduction

Graphene strip gratings may be used in antennas systems, frequency selective surfaces, tunable absorbers, sensors and plasmon waveguides [1-3]. Ultra high speed terahertz devices based on graphene have been already proposed and demonstrated [4]. In the THz range, the sensing application of graphene based on associated plasmon resonances is discussed in [5]. In periodic graphene strip grating, plasmon excitations and the plasmon resonance can be tuned by adjusting strip width and electrostatic doping over a broad THz range [6]. These properties led to designing of novel tunable antennas. One may control the electrodynamic characteristics of the whole grating using the static electric field and in such way changing the conductivity by varying chemical potential [7].

Multilayer graphene structures are well studied in optical range. In [8], [9], graphene photonic crystals are proposed. Graphene is modeled as a thin layer with certain permittivity. The error of such approach as well as application of the finite element method, finite-difference time-domain method, method of moments is discussed in [10].

In [11], diffraction by an infinite graphene periodic strip grating under normal incidence is considered with the use of the Fourier expansion method. The strict analysis of the same grating under arbitrary incidence with the use of the method of analytical regularization is given in [12]. In a subsequent paper [13], infinite periodic grating embedded in the dielectric slab is considered. In [14], the finite grating is considered. The problem is reduced to the hyper-singular integral equation.

Here, in this report, we are going to present rigorous approach to analyze gratings of graphene strips. In [15], we considered single layer of graphene with the use of the method of singular integral equations. Here we will extend this approach to the double layer graphene grating. Unlike commercial packages based on the finite-difference method or finite-element method, we take radiation conditions into account analitically, and do not rely on the appropriate choose of the basic functions as in the method of moments.

2. The Problem Statement

Consider *H*- polarized wave diffraction by two identical finite graphene periodic strip gratings. The strips width is $2d$. Denote the set of strips is every layer as $L=\bigcup_{m=1}^{M}(-d+l\cdot m;d+l\cdot m)$, where l is period, M is the number of strips in every layer. The distance between gratings is h (see Figure 1).

Total field we represent as a sum of the incident and scattered fields. It must satisfy the Helmholtz equation of the strips and the following boundary conditions:

$$\frac{1}{2}\left(E_y^+ + E_y^-\right)=\frac{1}{\sigma}\left(H_x^+ - H_x^-\right), \qquad (1).$$

$$E_y^+ = E_y^-,\ z=0. \qquad (2).$$

The tangential components of electric and magnetic fields are connected by the formula

$$E_y = -\frac{1}{i\omega\varepsilon_0}\frac{\partial H_x}{\partial z}. \qquad (3).$$

Sign "+" corresponds to the field above the grating, and sign "-" to the field below the grating. Graphene conductivity σ we obtain using Kubo formalism.

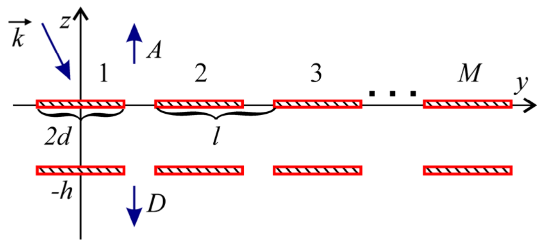

Figure 1. Structure geometry.

Represent scattered field as follows

$$H_x^r = \int_{-\infty}^{\infty} A(\xi)\exp(ik\xi y + ik\gamma(\xi)z)\ ,\ z>0\ , \quad (4).$$

$$H_x^s(y,z) = \int_{-\infty}^{\infty} C(\xi)\exp(ik\xi y - ik\gamma(\xi)z)d\xi + \int_{-\infty}^{\infty} B(\xi)\exp(ik\xi y + ik\gamma(\xi)(z+h))d\xi, \quad -h<z<0, \quad (5).$$

$$H_x^t(y,z) = \int_{-\infty}^{\infty} D(\xi)\exp(ik\xi y - ik\gamma(\xi)(z+h))d\xi, \quad z<-h\ , \quad (6).$$

where $\gamma(\xi)=\sqrt{1-\xi^2}$, $\operatorname{Re}\gamma \ge 0$, $\operatorname{Im}\gamma \ge 0$. In the following section we write integral equations relatively unknown spectral functions of the scattered field. Then, we reduce them to the system of singular integral equations.

3. Integral Equations

Unknown spectral functions in (4)-(6) are connected by the expressions which follow from (2)

$$A(\xi) = B\exp(ik\gamma(\xi)h) - C(\xi)\ , \quad (7).$$
$$D(\xi) = C(\xi)\exp(ik\gamma(\xi)) - B(\xi)\ .$$

From (1)-(3), (7) connected integral equations may be obtained

$$\int_{-\infty}^{\infty}\left(B(\xi) \pm C(\xi)\right)\exp(ik\xi y)d\xi = 0,\ \ y \notin L, \quad (8).$$

$$\frac{2ik}{\sigma Z}\int_{-\infty}^{\infty}\left(B(\xi) \pm C(\xi)\right)\exp(ik\xi y)d\xi + ik\int_{-\infty}^{\infty}\left(B(\xi) \pm C(\xi)\right)\gamma(\xi) \times \left(1 \mp \exp(ik\gamma(\xi)h)\right)\exp(ik\xi y)d\xi = -\frac{\partial}{\partial z}H^i(y,-h) \pm \frac{\partial}{\partial z}H^i(y,0),\ \ y \in L, \quad (9).$$

where $H^i(y,z)$ is incident field, Z is the free space impedance.

To reduce (8), (9) to the system of singular integral equations let us introduce functions [16]

$$F^{\pm}(y) = \int_{-\infty}^{\infty} ik\xi\left(B(\xi) \pm C(\xi)\right)\exp(iky\xi)d\xi. \quad (10).$$

If $F^{\pm}(y)$ are known then functions $B(\xi)$ and $C(\xi)$ may be obtained as inverse Fourier transform from (10).

In (9), function $\gamma(\xi) \sim i|\xi| + O(1/\xi)$ is increasing when $\xi \to \infty$. Let us represent it as $\gamma(\xi) = (\gamma(\xi) - i|\xi|) + i|\xi|$. Then $(\gamma(\xi) - i|\xi|) \to 0$, when $\xi \to \infty$. So, integrand in (9) may be represented as a sum of non-vanishing and vanishing functions. We use Hilbert transform

$$\mathrm{P}G(y) = \frac{1}{\pi}PV\int_{-\infty}^{\infty}\frac{G(\xi)}{\xi - y}d\xi\ , \quad (11).$$

$$\mathrm{P}\exp(ik\zeta y) = i\,\mathrm{sgn}(k\zeta)\exp(ik\zeta y)$$

to the non-vanishing term. $G(\xi)$ is an arbitrary function in (11), PV means Cauchy principal value integral. After that, non-vanishing terms in (9) will be transformed to the singular integrals, and vanishing terms using (10) will be transformed to the regular ones. Regular terms will be collected in the kernel function. As a result, the following system of singular integral equations with addition conditions may be obtained

$$\frac{1}{\pi}PV\int_L \frac{F^{\pm}(\xi)}{\xi - y}d\xi + \frac{1}{\pi}\int_L F^{\pm}(\xi)K^{\pm}(y,\xi)d\xi = -\frac{\partial}{\partial z}H_x^i(y,-h) \pm \frac{\partial}{\partial z}H_x^i(y,0),\ \ y \in L, \quad (12).$$

$$\frac{1}{\pi}\int_{-d+lm}^{d+lm} F^{\pm}(\xi)d\xi = 0\ ,\ \ m = 1,\,2,\,\ldots,M\ . \quad (13).$$

The kernel functions $K^{\pm}(y,\xi)$ are

$$K^{\pm}(y,\xi) = k\int_0^{\infty}\frac{\sin(k\zeta(y-\xi))}{\zeta}(\zeta + i\gamma(\zeta))d\zeta \mp ik\int_0^{\infty}\frac{\sin(k\zeta(y-\xi))}{\zeta}\gamma(\zeta)\exp(ik\gamma(\zeta)h)d\zeta + q(y,\xi), \quad (14).$$

$$q(y,\xi) = \begin{cases} \dfrac{2ik\pi}{\sigma Z}, & \xi \le y, \\ 0, & \xi > y. \end{cases} \quad (15).$$

Solution of (12)-(15) may be obtained by the method of discrete singularities [16]. The convergence is guaranteed by the theorems.

4. Numerical Results

It is convinient to use the total scattering cross-section (TSCS) and absorption cross-section (ACS) to study scattering and absorption characteristics,

$$TSCS = \frac{2\pi}{k}\int_0^{\pi}|A(-\cos\varphi)\sin\varphi|^2\ d\varphi + \frac{2\pi}{k}\int_{\pi}^{2\pi}|D(-\cos\varphi)\sin\varphi|^2\ d\varphi, \quad (16).$$

$$ACS = TSCS + \frac{4\pi}{k}\operatorname{Re}(D(-\cos\varphi_0))\ . \quad (17).$$

ACS is obtained from the power conservations law. Denote the chemical potential of graphene strip as μ_c. Suppose that plane wave with unit amplitude is incident on the grating. For all cases the relaxation time is $\tau = 1$ ps and room temperature $T = 300$ K.

The discretization of (12)-(13) is based on the Gauss-Chebyshev quadrature formulas of interpolation type with weight function. Denote the number of nodes on every strip as n. Figure 2 shows the convergence of the process, where $\varepsilon = \left|(TSCS(n) - TSCS(2n))/TSCS(2n)\right|$ is relative error of the TSCS. With parameter n increase, the error vanishes.

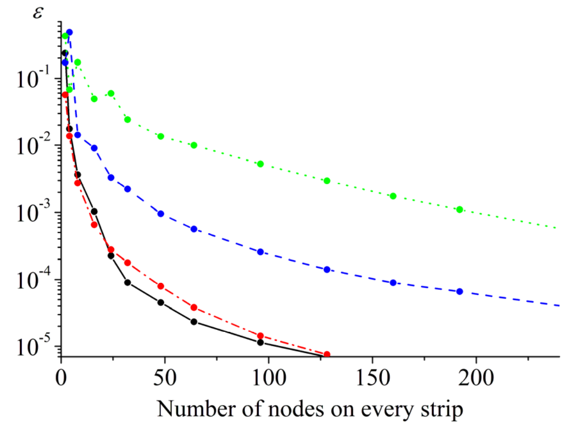

Figure 2. Relative error of the TSCS vs. number of nodes on every strip for two strips placed in parallel planes, $f = 1$ THz, $h = 30\mu\text{m}$ (black line), $f = 1$ THz, $h = 10\mu\text{m}$ (red line), $f = 4$ THz, $h = 30\mu\text{m}$ (blue line), $f = 5$ THz, $h = 30\mu\text{m}$ (green line), $d = 10\mu\text{m}$.

It is known that the first plasmon resonance frequency is about $f \approx 1.9$ THz for $\mu_c = 0.2$ eV, and $f \approx 2.6$ THz for $\mu_c = 0.4$ eV, $d = 10\mu\text{m}$ and $l = 40\mu\text{m}$. Let us take frequency within this frequency band and study scattering and absorption characteristics as functions of the distance between layers. Figure 3 shown dependences of TSCS and ACS vs. h for $f = 2$ THz. As it is usual at layered structures the bands of transparency and opacity appear. One may observe clearly seen maxima near resonances of the layered structure.

Let us now study characteristics of the grating for fixed values of h as functions of frequency. Figure 4 shows dependences of TSCS and ACS vs. f for two values of $h = 20\mu\text{m}$ and $h = 52\mu\text{m}$. Value $h = 52\mu\text{m}$ corresponds to the first resonance of layered structure for $\mu_c = 0.4$ eV and $f = 2$ THz. The opacity band near $f = 2$ THz appears due to two resonances: layered structure resonance and plasmon resonance.

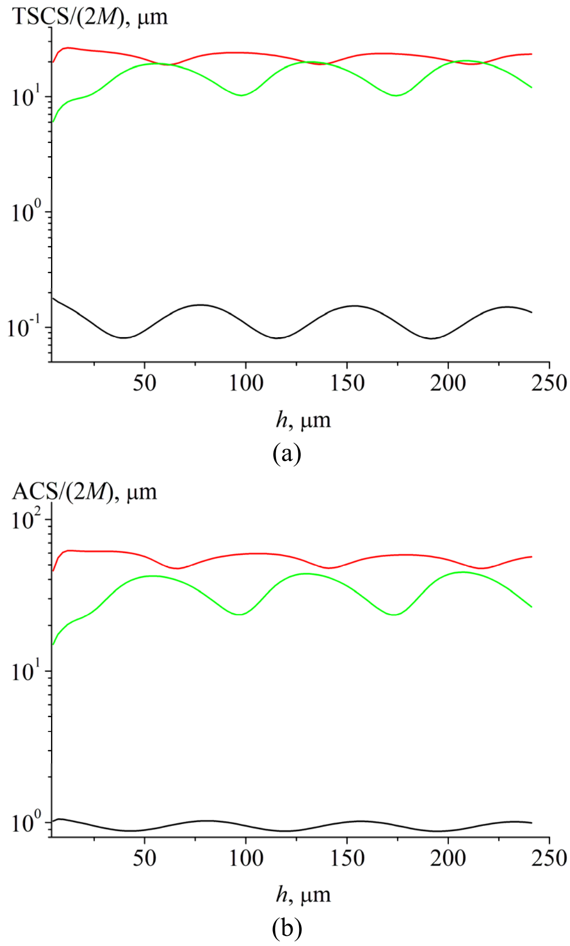

Figure 3. Dependences of TSCS (a) and ASC (b) vs. h for $\mu_c = 0$ eV (black line), $\mu_c = 0.2$ eV (red line), and $\mu_c = 0.4$ eV (green line), $d = 10\mu\text{m}$, $l = 40\mu\text{m}$, $M = 5$.

5. Conclusion

The rigorous solution of diffraction by the double layer graphene grating was obtained here by the method of singular integral equations. We studied the scattering and absorption characteristics for different values of chemical potential and distance between layers. The presented dependences demonstrate a variety of surface plasmon resonances and resonances of a layered structure in the THz range.

6. References

1. T. Otsuji, S. A. Boubanga Tombet, A. Satou, H. Fukidome, M. Suemitsu, E. Sano, V. Popov, M. Ryzhii, and V. Ryzhii, “Graphene-based devices in terahertz science and technology, ” *J. Phys. D: Appl. Phys.*, **45**, 30, 2012, 303001. doi: 10.1088/0022-3727/45/30/303001.

2. P. A. Huidobro, M. Kraft, R. Kun, S. A. Maier, J. B. Pendry, “Graphene, plasmons and transformation optics,” *Journal of Optics*, **18**, 4, 2016, 044024, doi: 10.1088/2040-8978/18/4/044024.

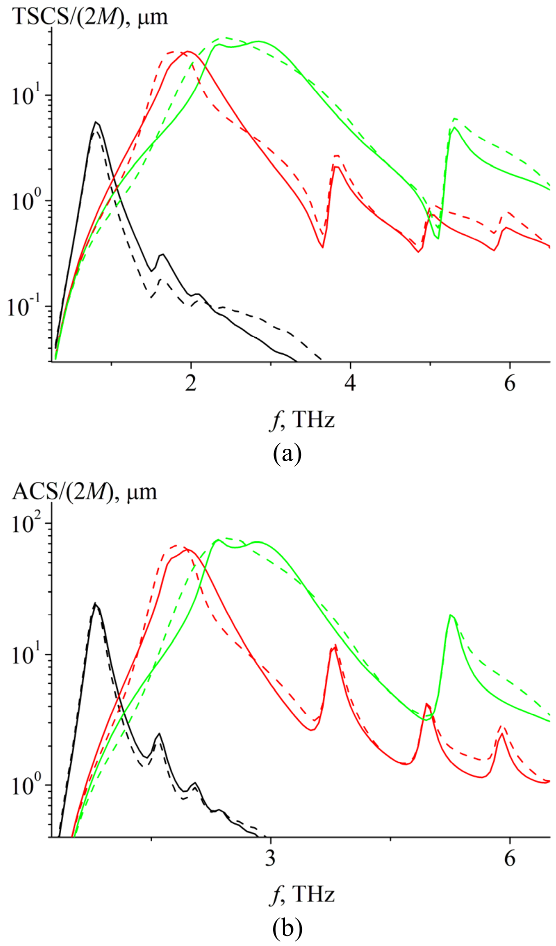

Figure 4. Dependences of TSCS (a) and ASC (b) vs. f for $\mu_c = 0$ eV (black lines), $\mu_c = 0.2$ eV (red lines), and $\mu_c = 0.4$ eV (green lines), $h = 20\mu\text{m}$ (solid lines), and $h = 52\mu\text{m}$ (dashed lines), $d = 10\mu\text{m}$, $l = 40\mu\text{m}$, $M = 5$.

3. J. M. Jornet, I. F. Akyildiz, "Graphene-based plasmonic nano-antenna for terahertz band communication in nanonetworks," *IEEE Journal on Selected Areas in Communications*, **31**, 12, 2013, pp. 685-694, doi: 10.1109/JSAC.2013.SUP2.1213001.

4. V. Ryzhii. "Terahertz plasma waves in gated graphene heterostructure,"*Japanese Journal of Applied Physics*, **45**, 33-36, 2006, pp. L923–L925, doi: 10.1143/JJAP.45.L923.

5. O. V. Shapoval, A. I. Nosich, "Bulk refractive-index sensitivities of the THz-range plasmon resonances on a micro-size graphene strip," *Journal of Physics D: Applied Physics*, **49**, 5, 2016, 055105/8, doi: 10.1088/0022-3727/49/5/055105.

6. L. Ju, B. Geng, J. Horng, C. Girit, M. Martin, Z. Hao, H. Bechtel, X. Liang, A. Zettl, Y. R. Shen, F. Wang, "Graphene plasmonics for tunable terahertz metamaterials," *Nature Nanotechnology*, **10**, 6, 2011, pp. 630-634, doi: 10.1038/nnano.2011.146.

7. K. Geim, K. S. Novoselov, "The rise of graphene," *Nature Materials*, **6**, 2007, pp. 183-191, doi:10.1038/nmat1849.

8. O. L. Berman, V. S. Boyko, R. Y. Kezerashvili, A. A. Kolesnikov, Y. E. Lozovik, "Graphene-based photonic crystal," *Physics Letters A*, **374**, 47, 2010, pp. 4784-4786, doi: 10.1016/j.physleta.2010.09.064.

9. O. A. Golovanov, G. S. Makeeva, V. V. Varenitsa, "Electrodynamic calculation of transmission coefficients for TEM-wave through the multilayer periodic graphene-dielectric structures at teraherz frequency range," *University proceedings. Volga region*. **32** , 4, 2014, no. 4, pp. 108-122.

10. Y. Shao, J. J. Yang, M. Huang, "A review of computational electromagnetic methods for graphene modeling," *International Journal of Antennas and Propagation*, **2016**, 2016, 7478621, doi: 10.1155/2016/7478621.

11. A. Y. Nikitin, F. Guinea, F. J. Garcia-Vidal, L. Martin-Moreno, "Surface plasmon enhanced absorption and suppressed transmission in periodic arrays of graphene ribbons," *Physical Review B*, **85**, 2012, 081405(R)/4, doi: 10.1103/PhysRevB.85.081405.

12. T. L. Zinenko, "Scattering and absorption of terahertz waves by a free-standing infinite grating of graphene strips: analytical regularization analysis," *Journal of optics*, **17**, 5, 2015, no. 5, pp. 1-8, doi: 10.1088/2040-8978/17/5/055604.

13. T. L. Zinenko, A. Matsushima, A. I. Nosich, "Surface-Plasmon, Grating-Mode, and Slab-Mode Resonances in the H- and E-Polarized THz Wave Scattering by a Graphene Strip Grating Embedded into a Dielectric Slab," *IEEE Journal of Selected Topics in Quantum Electronics*, **23**, 4, 2017, pp. 4601809, doi: 10.1109/JSTQE.2017.2684082.

14. O. V. Shapoval, J. S. Gomez-Diaz, J. Perruisseau-Carrier, J. R. Mosig, A. I. Nosich, "Integral equation analysis of plane wave scattering by coplanar graphene-strip gratings in the THz range", *IEEE Transactions on Terahertz Science and Technology*, **3**, no 5, 2013, pp. 666-674, doi: 10.1109/TTHZ.2013.2263805.

15. M. E. Kaliberda, L. M. Lytvynenko, S. A. Pogarsky, "Modeling of Graphene Planar Grating in the THz Range by the Method of Singular Integral Equations," *Frequenz*, doi: 10.1515/freq-2017-0059.

16. A. A. Nosich, Y. V. Gandel, "Numerical analysis of quasioptical multireflector antennas in 2-D with the method of discrete singularities: E-wave case," *IEEE Transactions on Antennas and Propagation*, **55**, 2, 2007, pp. 399-406, doi: 10.1109/TAP.2006.889811.