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Analysis of the Surface Plasmon Resonances of a Graphene Disk Stack: A Guaranteed and Fast Convergence Method

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Abstract

In this paper, the surface plasmon resonances of a graphene disk stack, excited by an impinging plane wave, are studied by means of the guaranteed and fast convergence Helmholtz-Galerkin technique. The surface plasmon resonance frequencies are individuated by the peaks of the absorption cross-section and the total scattering cross-section, which are expressed in closed form. It is shown that, for a graphene disk stack with a small distance between the disks compared to the disks radius, the plasmon mode resonance frequencies up-shift as the number of disks increases.

1. Introduction

The planar monolayer of carbon atoms organized in a honeycomb lattice, commonly referred to as graphene, is of great interest for the scientific community due to its optical, mechanical, thermal, and electronic properties, which make it a promising material for the development of various devices [1]. Among the others, particularly interesting is the ability of the graphene to support the propagation of surface plasmon polaritons in the terahertz and infrared spectrum with moderate losses, strong wave localization, and tunability [2]. As a result, a graphene disk is characterized by the surface plasmon resonances (SPRs), formed as Fabry–Perot-like standing waves due to the reflection of the surface plasmon polaritons at the disk rim, which can be tuned by applying an electrostatic/magnetostatic biasing field [3]. Moreover, in a graphene disk stack, for sufficiently small distance between the disks compared to the disks radius, the coupling between the surface plasmons originates the hybridization of the resonance modes, which, in turn, leads to the resonance frequencies shift [4].

From an electromagnetic point of view, a graphene object can be treated as an impedance surface and the corresponding impedance level can be obtained from the surface conductivity provided by the Kubo formalism [5]. As a result, a uniquely solvable boundary value problem for the Maxwell equations can be obtained by imposing the impedance boundary condition, the radiation condition, and the power boundedness condition. A classical way to solve this problem consists in resorting it to an equivalent singular integral equation for the surface current density [6]. Two problems arise: 1) Due to the singular nature of the obtained integral equation, only the uniqueness of the solution can be stated; 2) Even in case of existence of the solution, the discretization and truncation of the integral equation result in approximate solutions whose convergence to the exact solution of the problem is not guaranteed. Such problems can be overcome by means of the methods of analytical regularization, i.e., by recasting the obtained integral equation to a Fredholm equation of the second kind [7].

The aim of this paper is the analysis of the SPRs of a graphene disk stack excited by an incidence plane wave by means of the Helmholz-Galerkin method, belonging to the class of the methods of analytical preconditioning [7], introduced by the author for the analysis of PEC, resistive and graphene disks [8-14]. Such a method combines the analytical regularization and the discretization of the integral equation in a single step, i.e., the resulting matrix equation is of the Fredholm second kind. Moreover, the convergence is even fast because the selected expansion functions reconstruct the physical behaviour of the surface current densities. The resonance frequencies are individuated by the peaks of the absorption cross-section (ACS) and the total scattering cross-section (TSCS), admitting a closed form expression in terms of the surface current densities. It is shown that the SPR frequencies of a graphene disk stack with a small distance between the disks compared to the disks radius up-shift as the number of disks increases.

2. Formulation and Proposed Solution

A plane wave impinges onto a graphene disk stack realized by L equiaxial graphene disks with the same radius, a. According to the Kubo formalism [5], the surface conductivity, σ_s, can be expressed as in the following:

$$\sigma_s = \sigma_{intra} + \sigma_{inter}, \quad (1)$$

$$\sigma_{intra} = -j \frac{e^2 k_B T}{\pi\hbar^2\left(\omega - \frac{j}{t_{relax}}\right)} \left(\frac{\mu_c}{k_B T} + 2\, ln\left(e^{-\frac{\mu_c}{k_B T}} + 1\right)\right), \quad (2)$$

$$\sigma_{intra} = -j \frac{e^2\left(\omega - \frac{j}{t_{relax}}\right)}{\pi\hbar^2} \int_0^{+\infty} \frac{f_d(-\varepsilon) - f_d(\varepsilon)}{\left(\omega - \frac{j}{t_{relax}}\right)^2 - 4\left(\frac{\varepsilon}{\hbar}\right)^2} d\varepsilon, \quad (3)$$

$$f_d(\varepsilon) = \frac{1}{\left(e^{\frac{\varepsilon-\mu_c}{k_B T}}+1\right)}, \quad (4)$$

where k_0 is the free-space wavenumber, ω is the angular frequency, e is the electron charge, k_B is the Boltzmann constant, T is the temperature, $\hbar$ is the reduced Planck constant, t_{relax} is the relaxation time of an electron, and μ_c is the chemical potential. Let (ρ, ϕ, z) be a cylindrical coordinate system with the z axis orthogonal to the disks surfaces such that the i-th disk is located at the abscissa $z = z_i$.

By imposing the impedance boundary conditions on the disks surfaces, i.e.,

$$\hat{z} \times \left(\underline{E}(\rho, \phi, z_i^+) + \underline{E}(\rho, \phi, z_i^-)\right) \times \hat{z} = 2R\underline{J}_i(\rho, \phi) \quad (5)$$

for $\rho \leq a$, $0 \leq \phi < 2\pi$ and $i = 1,2, \ldots L$, where $\underline{E}(\cdot)$ denotes the total electric field, $\underline{J}_i(\cdot)$ is the surface current density on the i-th disk and $R = 1/\sigma_s$ is the surface resistivity of the disks, a boundary value problem for the Maxwell equations is obtained. According to the second Green formula, the problem can be formulated in terms of a system of L surface integral equations for the surface current densities [6]. By selecting the Green's function of the problem in order to automatically satisfy the radiation condition, and by properly defining the behaviour of the surface current densities at the disks rim in order to guarantee the finite energy in any bounded domain including the edge, the obtained system of integral equations admits a unique solution if it exists.

The revolution symmetry of the problem suggests expanding the fields in Fourier series. In this way, an equivalent formulation in terms of a system of L infinite sets of independent one-dimensional integral equations in the vector Hankel transform domain can be obtained [14], i.e., for the n-th azimuthal harmonic,

$$\sum_{j=1}^{L} \int_0^{+\infty} \underline{\boldsymbol{H}}^{(n)}(w\rho)\big(\underline{\widetilde{\boldsymbol{G}}}(w) - \delta_{i,j} R\underline{\boldsymbol{I}}\big)\underline{\tilde{\boldsymbol{J}}}_j^{(n)}(w) e^{-j|z_i - z_j|\sqrt{k_0^2 - w^2}} w dw = -\underline{\boldsymbol{E}}^{\mathrm{inc}(n)}(\rho, z_i) \quad (6)$$

for $\rho \leq a$ and $i = 1,2, \ldots L$, where $\underline{\boldsymbol{H}}^{(n)}(\cdot)$ is the kernel of the vector Hankel transform of order n (VHT$_n$), $\underline{\widetilde{\boldsymbol{G}}}(\cdot)$ is the spectral domain Green's function, $\underline{\boldsymbol{I}}$ is the identity operator, $\underline{\tilde{\boldsymbol{J}}}_i^{(n)}(\cdot)$ is the VHT$_n$ of the n-th harmonic of the surface current density on the i-th disk, and $\underline{\boldsymbol{E}}^{\mathrm{inc}(n)}(\cdot)$ is the n-th harmonic of the incident electric field.

The surface current densities can be represented as the superposition of a surface curl-free contribution and a surface divergence-free contribution [15]. The selection of such contributions as new unknowns has the advantage of being able to handle scalar unknowns in the spectral domain. Indeed, the VHT$_n$ of the n-th harmonic of such contributions have only one non-vanishing component [10], i.e.,

$$\underline{\tilde{\boldsymbol{J}}}_{i,C}^{(n)}(w) = \begin{pmatrix} \tilde{J}_{i,C}^{(n)}(w) \\ 0 \end{pmatrix}, \underline{\tilde{\boldsymbol{J}}}_{i,D}^{(n)}(w) = \begin{pmatrix} 0 \\ -j\tilde{J}_{i,D}^{(n)}(w) \end{pmatrix}, \quad (7)$$

where C and D identify the curl-free contribution and the divergence-free contribution, respectively. In order to discretize the equations in (6), Galerkin scheme is adopted. In this context, the scalar functions in (7) are expanded in the following series of weighted Bessel functions of the first kind [11]

$$\tilde{J}_{i,T}^{(n)}(w) = \sum_{h=-1+\delta_{n,0}}^{+\infty} \gamma_{i,T,h}^{(n)} \sqrt{2\eta_{T,h}^{(n)}} \frac{J_{\eta_{T,h}^{(n)}}(aw)}{w^{p_T}}, \quad (8)$$

where $T = C, D$, $\delta_{n,m}$ is the Kronecker delta, $\gamma_{i,T,h}^{(n)}$ denotes the general expansion coefficient, $\eta_{T,h}^{(n)} = |n| + 2h + p_T + 1$, $p_C = 3/2$, $p_D = 1$ and $J_n(\cdot)$ is the Bessel function of the first kind and order n [16], which constitute complete sets of orthonormal eigenfunctions of the most singular part of the integral operator reconstructing the physical behavior of the n-th harmonic of the surface current densities around the disks center and at the disks rim. As a result, the Galerkin projection acts as a perfect preconditioner and the general integral equation is recast as a fast-converging matrix equation of the Fredholm second kind. Moreover, the analytical technique proposed in [9] and [11] for the efficient evaluation of the matrix coefficients allows for very low computation time.

3. Numerical Results

The fast convergence of the proposed method, meaning that few expansion functions are needed to accurately reconstruct the solution with very low computation time, has been widely demonstrated in [8-14]. Hence, for the sake of brevity, this section is centered on the analysis of the SPRs of a graphene disk stack.

Let us consider L stacked graphene disks of radius $a = 50\mu\text{m}$, distance between the disks $d = z_{i+1} - z_i = 0.01a$ for $i = 1,2, \ldots L-1$, and the graphene conductivity taken for $T = 300K$, $t_{relax} = 1\text{ps}$ and $\mu_c = 1\text{eV}$. A plane wave orthogonally impinges onto the disk stack so that only the harmonics for $n = \pm 1$ contribute to the field reconstruction.

Figure 1 show ACS and TSCS, respectively, for varying values of the frequency in the terahertz range and for different numbers of disks involved. The SPR frequencies can be clearly identified by the peaks of ACS and TSCS. The black dotted lines in Figure 1, circling the peaks related to the same SPR, show that, for the case examined, the SPRs migrate to higher and higher frequencies as the number of disks involved is higher.

For the sake of completeness, Figure 2 show the behavior of the near total electric field in the plane containing the upper disk at the resonance frequencies 4.6371587THz for $L = 1$, 5.7825500THz for $L = 2$ and 6.3585366THz for $L = 3$, respectively, which are related to the same SPR. As can be clearly seen, the behavior is similar, however, some variations can be appreciated due to the disks coupling.

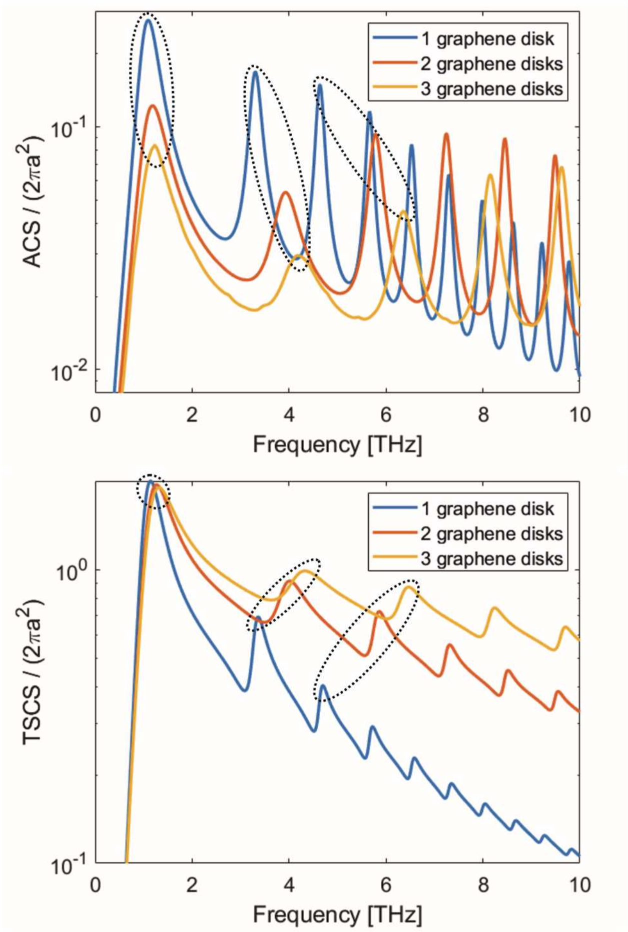
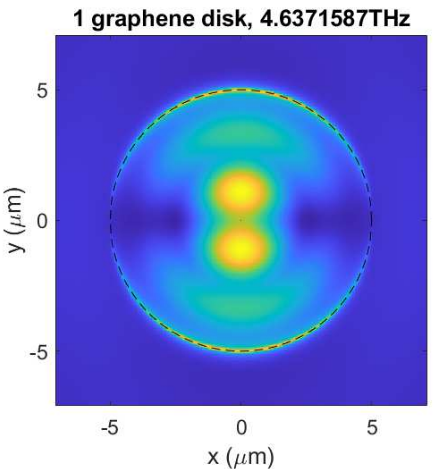


Figure 1. Normalized ACS and TSCS when a plane wave ortogonally impinges onto a graphene disk stack for varying values of the frequencies and for different numbers of the disks involved. $\boldsymbol{a} = \mathbf{50}$µm , $\boldsymbol{d} = \mathbf{0.01}\boldsymbol{a}$, $\boldsymbol{T} = \mathbf{300}\boldsymbol{K}$, $\boldsymbol{t_{relax}} = \mathbf{1}$ps and $\boldsymbol{\mu_c} = \mathbf{1}$eV.



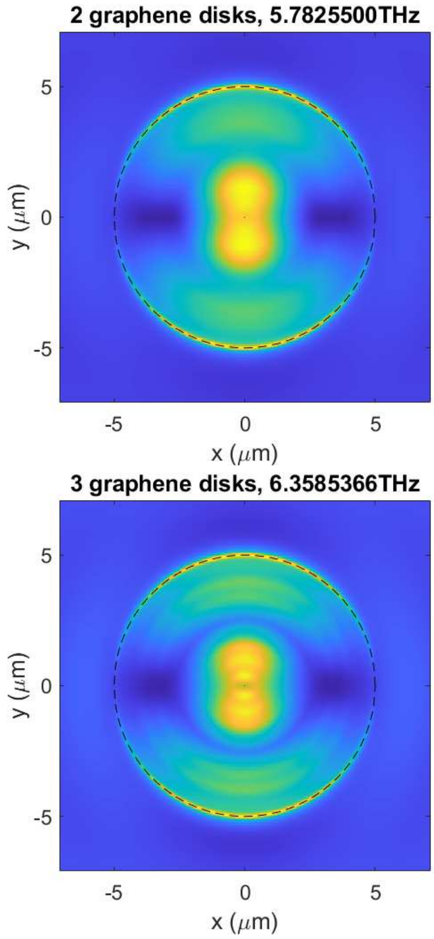


Figure 2. Near total electric field in the plane containing the upper disk of the graphene disk stack described in the caption of Figure 1 at the resonance frequencies 4.6371587THz for $\boldsymbol{L} = \mathbf{1}$, 5.7825500THz for $\boldsymbol{L} = \mathbf{2}$ and 6.3585366THz for $\boldsymbol{L} = \mathbf{3}$, related to the same SPR.

References

[1] A. Geim and K. Novoselov, "The Rise of Graphene," *Nature Mater*, **6**, 2007, pp. 183–191, doi:10.1038/nmat1849.

[2] A. Grigorenko, M. Polini, and K. Novoselov, "Graphene Plasmonics," *Nature Photon*, **6**, 2012, pp. 749–758, doi: 10.1038/nphoton.2012.262.

[3] M. V. Balaban, O. V. Shapoval, A. I. Nosich, "THz Wave Scattering by a Graphene Strip and a Disk in the Free Space: Integral Equation Analysis and Surface Plasmon Resonances," *Journal of Optics*, **15**, 2013, art. 114007, doi: 10.1088/2040-8978/15/11/114007.

[4] F. Ramirez, B. Liu, and S. Shen, "Extreme Blueshift of Surface Plasmon Resonance Frequency in Graphene Nanodisk Stacks," *Journal of Quantitative Spectroscopy & Radiative Transfer*, **158**, 2015, pp. 27–35. doi: 10.1016/j.jqsrt.2014.12.004.

[5] G. W. Hanson, “Dyadic Green’s Functions for an Anisotropic, Non-Local Model of Biased Graphene,” *IEEE Transactions on Antennas and Propagation*, 56, 2008, pp. 747–757, doi: 10.1109/TAP.2008.917005.

[6] 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**, 2013, pp. 666–674, doi: 10.1109/TTHZ.2013.2263805.

[7] A. I. Nosich, “Method of Analytical Regularization in Computational Photonics,” *Radio Science*, **51**, 2016, pp. 1421–1430, doi: 10.1002/2016RS006044.

[8] M. Lucido, G. Panariello, and F. Schettino, “Scattering by a Zero-Thickness PEC Disk: A New Analytically Regularizing Procedure Based on Helmholtz Decomposition and Galerkin Method,” *Radio Science*, **52**, 1, 2017, pp. 2–14, doi: 10.1002/2016RS006140.

[9] M. Lucido, F. Di Murro, and G. Panariello, “Electromagnetic Scattering from a Zero-Thickness PEC Disk: A Note on the Helmholtz-Galerkin Analytically Regularizing Procedure,” *Progress in Electromagnetics Research Letters*, **71**, 2017, pp. 7–13, doi: 10.1080/09205071.2017.1291364.

[10] M. Lucido, M. V. Balaban, S. Dukhopelnykov, and A. I. Nosich, “A Fast-Converging Scheme for the Electromagnetic Scattering from a Thin Dielectric Disk,” *Electronics*, **9**, 9, 2020, p. 1451 (12 pages), doi: 10.3390/electronics9091451.

[11] M. Lucido, F. Schettino and G. Panariello, “Scattering from a Thin Resistive Disk: A Guaranteed Fast Convergence Technique,” *IEEE Transactions on Antennas and Propagation*, **69**, 1, 2021, pp. 387–396, doi: 10.1109/TAP.2020.3008643.

[12] M. Lucido, M. V. Balaban, and A. I. Nosich, “Plane Wave Scattering from Thin Dielectric Disk in Free Space: Generalized Boundary Conditions, Regularizing Galerkin Technique and Whispering Gallery Mode Resonances,” *IET Microwave, Antennas & Propagation*, **15**, 10, 2021, pp. 1159–1170, doi: 10.1049/mia2.12106.

[13] M. Lucido, “Electromagnetic Scattering from a Graphene Disk: Helmholtz-Galerkin Technique and Surface Plasmon Resonances,” *Mathematics*, **9**, 2021, p. 1429 (15 pages), doi: 10.3390/math9121429.

[14] M. Lucido, “Analysis of the Scattering from a Two Stacked Thin Resistive Disks Resonator by Means of the Helmholtz–Galerkin Regularizing Technique,” *Applied Sciences,* **11**, 17, 2021, p. 8173 (16 pages). doi: 10.3390/app11178173.

[15] J. Van Bladel, “A Discussion of Helmholtz’ Theorem on a Surface,” *AEÜ*, **47**, 1993, pp. 131–136, doi: 10.1080/02726349308908332.

[16] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*; Verlag Harri Deutsch: Frankfurt, Germany, 1984.