Numerical Model and Analysis of a Graphene Periodic Structure

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Abstract— The aim of this paper is to present the particulars of new research in special numerical models of structures used for nano-applications. These models can be advantageously used in the evaluation of electromagnetic parameters, thus helping researchers and designers to solve problems related to nanoelements and nanotechnology. The first numerical model of large periodic structure is designed to test electromagnetic wave propagation in a graphene composite structure. There are the results of a numerical analysis of simple nano-electric line.

1. INTRODUCTION

According to the research presented in papers [1, 3], the periodic structure of graphene exhibits certain interesting electrical and electromagnetic properties regarding the propagation of an electromagnetic (EMG) wave. The referenced articles nevertheless do not provide a clear conclusion that would facilitate prospective application of periodic structures with extreme properties in the field of EMG wave propagation; these structures can be based on either natural or artificial materials. The authors proposed analysis has to be built upon a specific numerical model; this model should respect the character of the Telegrapher's equations as well as the multiplicity of the repeating periodic structure element [5].

2. MODEL OF A PERIODIC STRUCTURE

The geometrical model is shown in Figs. 1(a), (b). For any case of analysis of transient processes in the quantum physics particle position shift, the model according to Formula (1) is suitable for the description of transient processes of dynamically assumed particles [2]. The model with a higher order of the time variation of the functional u, namely the model described by the Telegrapher's equation, is expressed in the form

$$\Delta u = C_{t0}\frac{\partial^2 u}{\partial t^2} + C_{t1}\frac{\partial u}{\partial t} + C_{t2}u + C_{t3}. \tag{1}$$

The proposed numerical model is based on the formulation of partial differential equations for the EMG field, known as reduced Maxwell's equations; according to Heaviside's notation, we have the following formula for the magnetic field intensities and flux densities:

$$\mathrm{rot}\mathbf{E} = -\frac{\partial\,\mathbf{B}}{\partial\,t} + \mathrm{rot}\,(\mathbf{v}\times\mathbf{B})\,, \quad \mathrm{rot}\mathbf{H} = \mathbf{J}_T + \frac{\partial\mathbf{D}}{\partial t} + \mathrm{rot}\,(\mathbf{v}\times\mathbf{D}) \tag{2}$$

$$\mathrm{div}\,\mathbf{B} = 0, \quad \mathrm{div}\,\mathbf{D} = \rho, \tag{3}$$

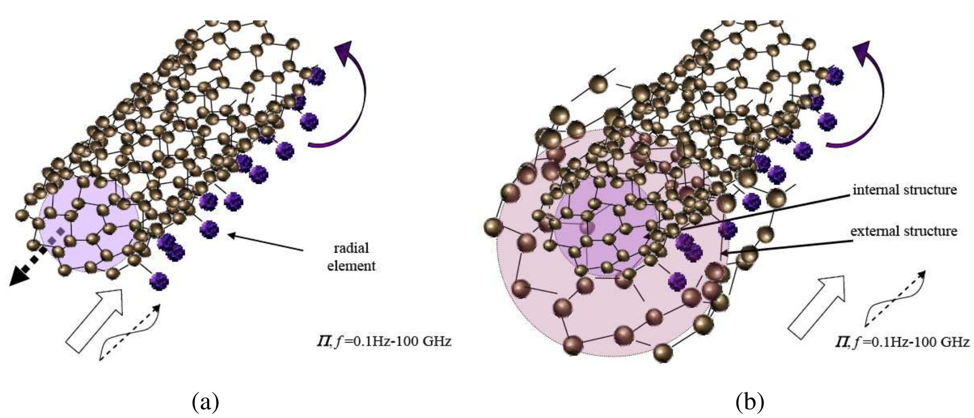


Figure 1: A geometrical structure of the numerical analysis of surface wave propagation: (a) single wire; (b) coaxial line.

where $\mathbf{H}$ is the magnetic field intensity, $\mathbf{B}$ is the magnetic field flux density, $\mathbf{J}_T$ is the total current density, $\mathbf{D}$ is the electric flux density, $\mathbf{E}$ is the electric field intensity, ρ is the electric charge volume density, $\mathbf{v}$ is the instantaneous velocity of the moving element. Respecting the continuity equation

$$\operatorname{div}\mathbf{J}_T = -\frac{\partial\rho}{\partial t}, \tag{4}$$

the vector functions are expressed by means of the scalar electric potential ϕ_e and the vector magnetic potential $\mathbf{A}$, and, after Coulomb calibration [4, 6, 8]. Considering the velocity of moving electrically charged particles $\mathbf{v}$ in the magnetic field, the total current density $\mathbf{J}_T$ from Formula (2) is

$$\mathbf{J}_T = \gamma\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right) - \frac{\partial\left(\varepsilon\mathbf{E}\right)}{\partial t} + \frac{\gamma}{q}\left(\frac{m\mathrm{d}\mathbf{v}}{\mathrm{d}t} + l\mathbf{v} + k\int_t \mathbf{v}\mathrm{d}t\right), \tag{5}$$

where m is the particle mass, where m_0 is the quiescent mass of the particle (7), (8), q is the electric charge of the moving particle, γ is the specific conductivity of the environment from the macroscopic perspective, l is the damping coefficient, and k is the stiffness coefficient of the surrounding environment. The material electromagnetic relations for the macroscopic part of the model are represented by the terms of symbolically isotropic properties

$$\mathbf{B} = \mu_0\mu_r\mathbf{H}, \quad \mathbf{D} = \varepsilon_0\varepsilon_r\mathbf{E}, \tag{6}$$

where the quantity indexes of the permeabilities and permittivities r denote the relative quantity value and 0 denotes the value of the quantity for vacuum. The relationship between the macroscopic and the microscopic parts of the model (particle dynamics in the electromagnetic field) [7, 11, 12] is described by the formulas defining the force acting on individual electrically charged particles of the electromagnetic field in their gravity centre, and the effect is considered of the motion of the electrically charged particles on the surrounding electromagnetic field:

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} + l\mathbf{v} + k\int_t \mathbf{v}\mathrm{d}t = q\ \left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right) - \frac{q}{\gamma}\frac{\partial\left(\varepsilon\mathbf{E}\right)}{\partial t}. \tag{7}$$

The relationship between the macroscopic model of the geometrical part of the electromagnetic field and the quantum-mechanical model of bound particles is expressed via the application of current density (5) and by the Formula (2) as follows:

$$\mathrm{rot}\mathbf{H} = \gamma\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right) - \frac{\partial\left(\varepsilon\mathbf{E}\right)}{\partial t} + \frac{\gamma}{q}\left(\frac{m_0\left(1-\frac{v^2}{c^2}\right)^{-\frac{1}{2}}\mathrm{d}\mathbf{v}}{\mathrm{d}t} + l\mathbf{v} + k\int_t \mathbf{v}\mathrm{d}t\right) + \frac{\partial\mathbf{D}}{\partial t} + \mathrm{rot}\left(\mathbf{v}\times\mathbf{D}\right) \tag{8}$$

With respect to the fact that the model comprises not only the electric and magnetic components of the EMG wave but also the space of the motion of the electrically charged particles, including the action of interacting forces, it is necessary to solve the model as a designed system (1). By applying the Galerkin method to find the functional minimum (as described in, for example, reference [9]) and considering the boundary conditions, we obtain the numerical model as a system of non-linear equations to be solved by standard methods.

3. DETAILED GEOMETRY OF THE MODEL OF A PERIODIC STRUCTURE

The design of the geometrical model can be characterized in greater detail as suggested in this section of the paper. The fundamental element of a graphene-based periodic structure is a "benzene" core; from the perspective of the stochastic distribution of the instantaneous position and arrangement of carbon C valence electrons, the fundamental element can be schematically described as shown in Fig. 4 [10].

The structure of the symmetrical configuration of graphene-based polymer tubes is then presented in Fig. 3. The diameter difference between both tubes corresponds to $\Delta D = 1\,\mathrm{nm}$, assuming the inner tube diameter of $D_1 = 5\,\mathrm{nm}$. In Figs. 2 and 3, we indicate hydrogen bonds in the polymer structure. In thus configured model with the stochastic presence of the instantaneous position of electron bonds, we have to evaluate the power flux along the polymer tubes. Fig. 4 shows a

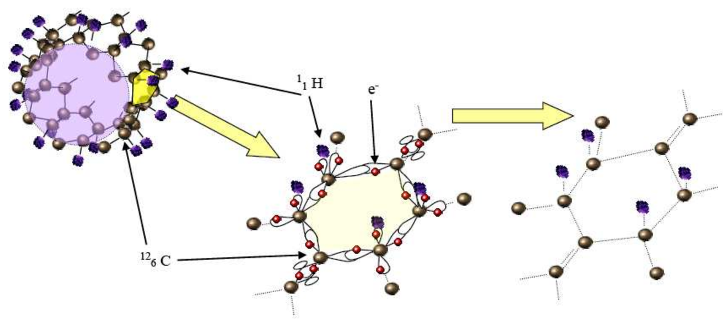


Figure 2: A geometrical model of the basic structure element with the probabilistic distribution of valence electrons.

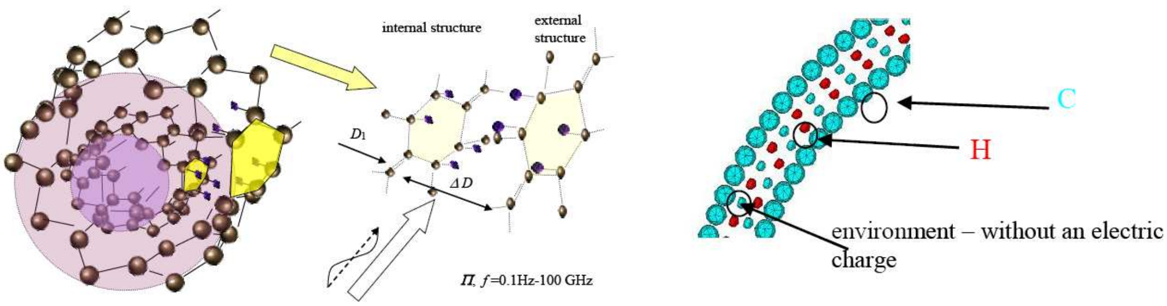


Figure 3: A coaxial line model tested for the passage of the active power Π flux density.

geometrical model to evaluate the power density propagation, with the instantaneous value of the Poynting vector expressed within the formula

$$\mathbf{\Pi}(t) = \mathbf{E}(t) \times \mathbf{H}(t) \tag{9}$$

It is obvious from the above Formula (9) that the resulting values of the Poynting vector depend on the instantaneous values of the $\mathbf{E}(t)$ and $\mathbf{H}(t)$.

The mathematical-numerical model [10] consists of basic elements [6] characterizing the ANSYS software, namely SOLID236 and SOLID226 [6] and others, and it is complemented with the proper code of the model according to Formulas (6), (7), and (8).

4. SETTING THE BOUNDARY CONDITIONS

The basic formation (an element of the periodic structure) can be simply described by atom bonds, namely motion of the valence electrons (Fig. 4). Another step in setting the conditions of the model consists in evaluating the electric field $\mathbf{E}$ intensity vector of components in both the radial and the tangential direction, $\mathbf{E}_r$, $\mathbf{E}_t$, Fig. 3. We can — for the hydrogen atom H bound to carbon C and one binding electron for the middle electrodes of the coaxial arrangement of the internal structure (Fig. 4) — evaluate the radial electric field intensity from the single bond C–H as

$$\begin{aligned} E_{r,a} &= \frac{1}{4\pi\varepsilon_0} \cdot \frac{q_e}{|R_a|^2}, \\ E_{r,a} &= \frac{1}{4\pi \cdot 8.856 \cdot 10^{-12}} \cdot \frac{1.602 \cdot 10^{-19}}{1.14 \cdot 10^{-10}} = \frac{1 \cdot 1.602}{4\pi \cdot 8.856 \cdot 1.14} \cdot 10^4 = 0.01263 \cdot 10^4 \,\mathrm{V/m} \end{aligned} \tag{10}$$

Based on the knowledge of the microscopic model, it is then possible to evaluate the macroscopic parameters, such as the specific conductance γ, the magnetic susceptibility χ, the magnetic permeability μ, or the electric permittivity ε of the environment. From the differential form of Ohm's law for example, we can write the flux density.

$$\mathbf{J} = \overset{\leftrightarrow}{\gamma} \cdot \mathbf{E}, \tag{11}$$

where $\overset{\leftrightarrow}{\gamma}$ is the specific conductance tensor.

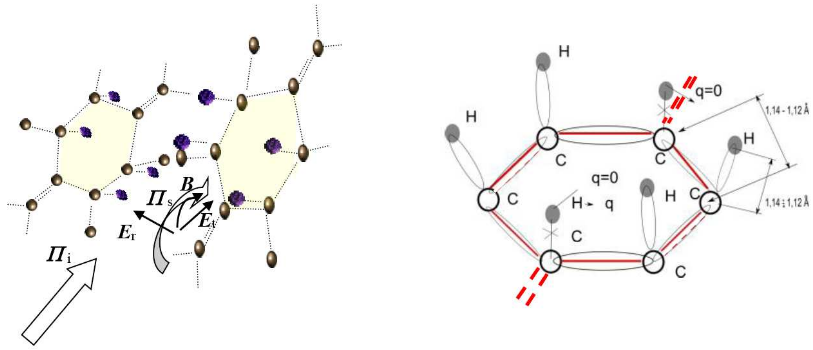


Figure 4: A model of the basic element of the periodic structure of the model based on graphene polymer.

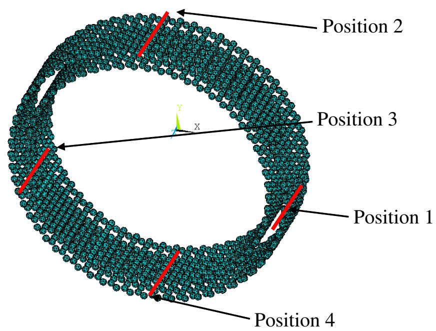
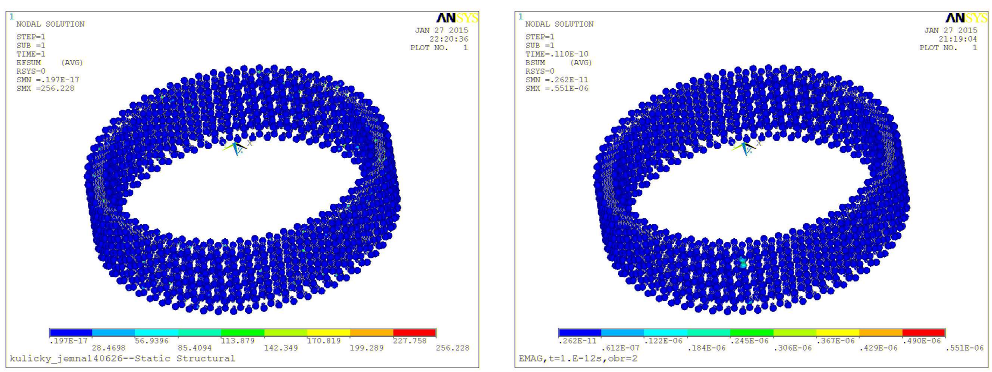
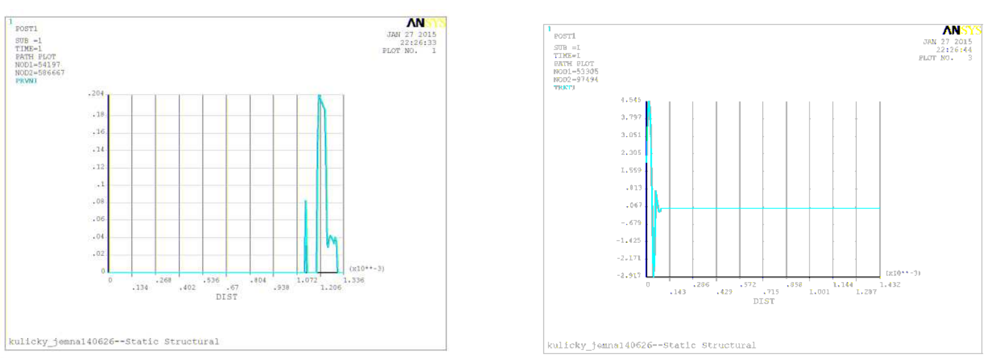


Figure 5: A geometrical model and curves 1, 2, 3 and 4 for the Poynting vector evaluation.



(a) (b)

Figure 6: The distribution of (a) the electric field intensity module $E(t)$ [V/μm], $t_1 = 1\,\mathrm{ps}$, (b) of the magnetic flux density module $B(t)$ [pT], $t_1 = 1\,\mathrm{ps}$.



(a) (b)

Figure 7: The behaviour of the distribution of the power specific density module $\Pi(t)$ [pW/μm^2], $t_1 = 1\,\mathrm{ps}$ (a) along curve 1, (b) along curve 3.

5. RESULTS OF THE NUMERICAL MODEL

The results of the analysis of the numerical model are shown as the distribution of the intensities and flux of the electric and magnetic quantities, Fig. 6, further, the results are also indicated as the distribution of the instantaneous Poynting vector components (Fig. 7) along the curves 1 to 4 from Fig. 5. for current excitation in an electric line $i(t) = I * f(t)$, where $I = 1\,\mu\mathrm{A}$.

6. CONCLUSION

We designed a geometrical model of a nanostructure exhibiting a high rate of periodicity, and we also designed a numerical model for the solution and analysis of effects occurring in the propagation of an EMG wave along the nanostructure. Initial numerical experiments targeting the propagation of and EMG wave in the nanostructure were performed to complete the set of research activities.

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