Numerical Model of a Large Periodic Structure

R. Urban, P. Drexler, P. Fiala, and D. Nešpor
FEEC, BUT, UTEE, Technická 12, Brno 616 00, Czech Republic

Abstract— The aim of this paper is to present the particulars of new research in special numerical models of structures used for nanoapplications. 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. According to the interpretation of the results, the basic design will be prepared for experimental fabrication of the functional sample.

1. INTRODUCTION

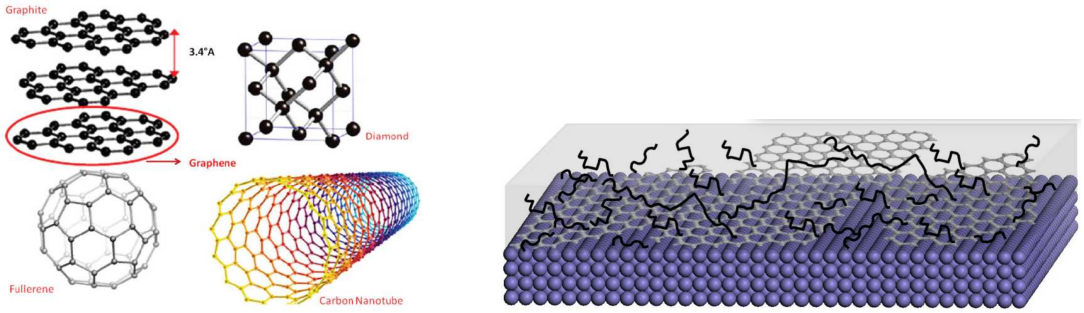
It is obvious from the research presented in papers [1, 3] that the periodic structure of graphene should exhibit certain interesting electrical and electromagnetic properties regarding the propagation of an electromagnetic wave. Thus, new horizons could be opened for the use of graphene in electrical engineering (EMG) and electronics. 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 electromagnetic wave propagation; these structures can be based on either natural or artificial materials.

The authors of this paper have developed the idea to set up a simple numerical model and to propose an experiment suitable for the related verification. Fig. 1 shows the known concepts of carbon nanostructures [2, 3] and layered polymer. The numerical model enables us to evaluate the propagation of an electromagnetic wave along the surface consisting of a periodic structure (such as graphene or metamaterial) and the surrounding dielectric environment The aim of the model is to evaluate the components of both the EMG wave and the power flux density in the time domain; thus, based on our knowledge of today's manufacturing technologies, it would be easily possible to define the applicability of the periodic structure for specific purposes in electrical engineering and electronics. Examples of periodic structure arrangements can be found in several studies, for instance in the referenced paper [2], Fig. 2.

The proposed analysis has to be based on 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.

2. MODEL OF A PERIODIC STRUCTURE

The geometrical model designed to provide a simple comparison between classic materials and those based on a periodic structure with a large number of repeated elements could be identified with the body shown in Fig. 3. The presented drawing shows the concept of a macroscopic approach to the model combined with a quantum-mechanical model, both of which are described by concentric



(a) (b)

Figure 1: Structures of carbon nanomaterials [2, 3]: (a) known arrangement of carbon structures; (b) graphene-polymer composite.

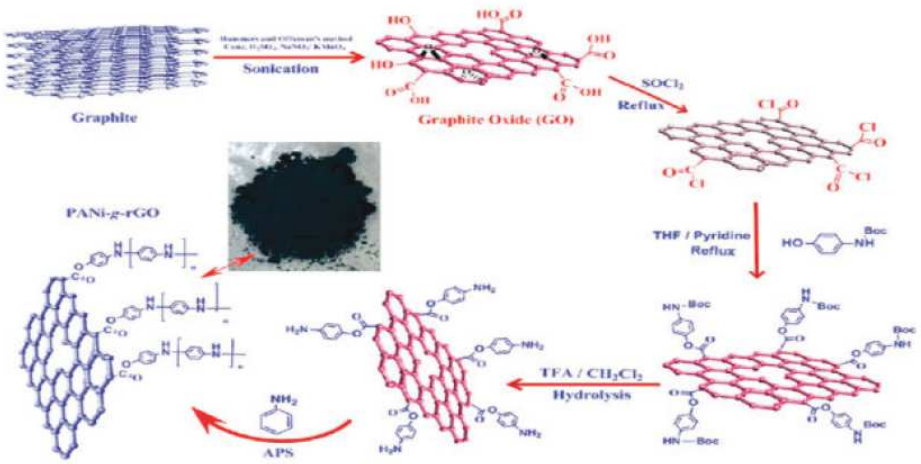


Figure 2: Formation of a special graphene-polymer structure (composite) [2].

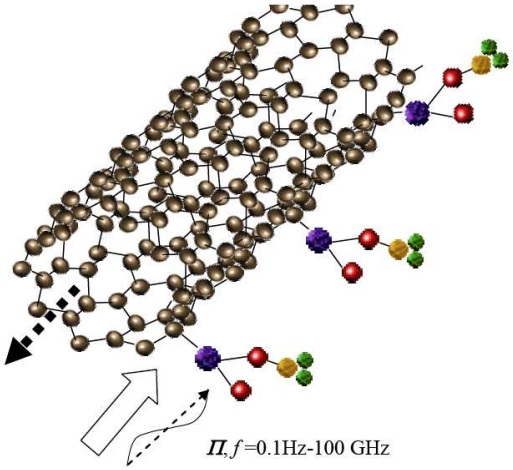


Figure 3: Geometrical structure of the numerical analysis of surface wave propagation.

particles. In a radial coordinate, the model will assume dimensions in the order of nanometers, and in the longitudinal axis the dimensions will be more than several tens of millimeters.

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

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

This model represents precisely the dynamics of the system of moving particles, and the simplified form of the model is the well-known wave equation in the form

$$\Delta u = C_{w0}\frac{\partial^2 u}{\partial t^2} \tag{2}$$

The above-described hypothesis based on formula (1) and coupled with relation (2) offers an easier solution — albeit of a more complicated model — using the numerical apparatus. The solution consists in a periodic damped wave written generally as

$$u = C_{tv1}e^{F(t)}e^{F(\Omega)} \tag{3}$$

where Ω is the space for which relation (1) was formulated. As a result of the proposed model, there occurs a shift in the field of quantum physics. Based on relations (1) and (2), it is possible to assume that the elementary phenomenon of the quantum physics solution is an electromagnetic wave. A particle (plasmon), according to the hitherto used quantum physics hypothesis, is the result of the waves‘ interference effect. It is assumed that the basic elements of matter are an electric charge and its motion. The fundamentals of this hypothesis have been already described in papers and reports [5, 7], proposing that

$$\rho_e^2 = \rho_g \tag{4}$$

where ρ_e is the electric charge volume density and ρ_g is the volume density of matter.

The model (1), (2) enables us, using the well-known numerical methods, to simulate the behaviour of the individual basic types and geometries of elements of nanomaterial and periodic structures.

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

$$\mathrm{rot}\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} + \mathrm{rot}\left(\mathbf{v} \times \mathbf{B}\right), \quad \mathrm{rot}\mathbf{H} = \mathbf{J}_T + \frac{\partial \mathbf{D}}{\partial t} + \mathrm{rot}\left(\mathbf{v} \times \mathbf{D}\right) \tag{5}$$

$$\mathrm{div}\,\mathbf{B} = 0, \quad \mathrm{div}\,\mathbf{D} = \rho, \tag{6}$$

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

$$\mathrm{div}\,\mathbf{J}_T = -\frac{\partial \rho}{\partial t}, \tag{7}$$

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 [8], the relationship between the quantities is expressed as

$$\mathbf{E} = -\mathrm{grad}\phi_\mathrm{e} - \frac{\partial \mathbf{A}}{\partial t}, \tag{8}$$

$$\mathbf{B} = r\mathrm{ot}\mathbf{A}. \tag{9}$$

Considering the velocity of moving electrically charged particles $\mathbf{v}$ in the magnetic field, the total current density $\mathbf{J}_T$ from formula (5) is

$$\mathbf{J}_T = \gamma\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right) - \frac{\partial\left(\varepsilon \mathbf{E}\right)}{\partial t} + \frac{\gamma}{q}\left(\frac{m\mathrm{d}\mathbf{v}}{\mathrm{d}t} + l\mathbf{v} + k\int_t \mathbf{v}\mathrm{d}t\right), \tag{10}$$

where m is the particle mass, considering the formula

$$m = m_0\left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}}, \tag{11}$$

where m_0 is the quiescent mass of the particle, 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, 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

$$\mathbf{B} = \mu_0\mu_r\mathbf{H}, \quad \mathbf{D} = \varepsilon_0\varepsilon_r\mathbf{E}, \tag{12}$$

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) 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:

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} + l\mathbf{v} + k\int_t \mathbf{v}\mathrm{d}t = q\ (\mathbf{E} + \mathbf{v}\times\mathbf{B}) - \frac{q}{\gamma}\frac{\partial\left(\varepsilon\mathbf{E}\right)}{\partial t}. \tag{13}$$

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 (10) and by the formula (5) as follows:

$$\mathrm{rot}\mathbf{H} = \gamma(\mathbf{E} + \mathbf{v}\times\mathbf{B}) - \frac{\partial(\varepsilon\mathbf{E})}{\partial t} + \frac{\gamma}{q}\left(\frac{m_0\left(1-\frac{v^2}{c^2}\right)^{-\frac{1}{2}}\mathrm{d}\mathbf{v}}{\mathrm{d}t} + l\mathbf{v} + k\int_t \mathbf{v}\mathrm{d}t\right) + \frac{\partial\mathbf{D}}{\partial t} + \mathrm{rot}\left(\mathbf{v}\times\mathbf{D}\right). \tag{14}$$

With respect to the fact that the model comprises not only the electric and the magnetic components of the electromagnetic 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) characterised by the Telegrapher's equations.

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. The model is designed for the ANSYS software, where the solution is carried out with finite numerical methods [10].

3. THE STRUCTURE MODEL

As indicated above, the basic model is built in a system based on the finite element method, namely the ANSYS tool, and enables us to find the geometry and parameters of the target structure with respect to its chemical survivability. The elementary structure according to Fig. 2 was chosen and solved as the basis of the numerical model according to formula (14).

The geometry of a large system incompatible both in its dimensions and the number of included elements is solved with the known condition of periodicity and also as a partially stochastic model Certain problems occur in modelling the bond between the polymer and the graphene basis. The mathematical-numerical model consists of basic elements characterising the ANSYS software, namely HF119, HF120 and others, and it is complemented with the proper code of the model according to formula (14). Currently, the model solution process is at the stage of tuning and the related verification of the gradually obtained analytical result is being performed Considering the robustness of the model, it is necessary to point out that the making and analysis of the model are time-intensive activities.

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4. CONCLUSION

We designed the numerical model of a large periodic structure to analyse the propagation of an electromagnetic wave in such a structure. The model is currently under testing, and analyses of the results are being carried out. Simultaneously, we are designing an experiment to verify and compare the results obtained via examination of the model.

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