A Numerical Model of the Concept of a Graphene Polymer-Based Sensor

[2]M. Cap, [1]P. Fiala, [2]D. Nešpor, [1]P. Drexler

[1]SIX VUT v Brně, Technická 12, 616 00 Brno, Czech Republic,
[2]Department of Theoretical and Experimental Electrical Engineering, Technicka 12, 616 00 Brno, Czech Republic,
Email: capm@feec.vutbr.cz

Abstract. *The paper discusses the design and analysis of a graphene coaxial line suitable for sub-micron sensors of magnetic fields. The proposed numerical model is based on an analysis of a periodic structure with high repeatability, and it is built upon a graphene polymer having a basic dimension in nanometers. The model simulates the actual random motion in the structure as the source of spurious signals and considers the pulse propagation along the structure; furthermore, the model also examines whether and how the pulse will be distorted at the beginning of the electric line. The results of the analysis are necessary for further use of the designed sensing devices based on graphene structures.*

Keywords: Nanomaterials, Graphene, Signal sensing, Signal/Noise, Large periodic structure

1. Introduction

It is obvious from the research presented in papers [1] and [2] that the periodic structure of graphene should exhibit certain interesting electrical and electromagnetic properties regarding the propagation of an electromagnetic 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. The authors have developed the idea to set up a simple numerical model and to propose an experiment suitable for the related verification. 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 metamaterials) and the surrounding dielectric environment. Generally, 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. The model embodies an application of the quantum-mechanical model of matter and stochastic distribution of electric charge in individual elements of the structure. Although the structure is large, it exhibits a significant degree of periodicity; thus, it is possible to utilize, up to a certain level of complexity, the known finite methods (the finite and boundary element techniques or the finite volume method combined with a deterministic stochastic model, extreme modelling [3], [4]). An example is provided in Fig. 1a via the design of a single conductor with non-conductive surface, which represents the periodic structure of a graphene-based polymer or, by extension, a more complex application of such structure; to be more concrete, we can refer to Fig 1b and the model of a coaxial, symmetric electric line comprising two polymer systems formed on graphene basis.

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 is suitably expressed by the body shown in Fig. 1a, b. The presented drawing shows the concept of a macroscopic approach to the model combined with a quantum-mechanical model, both of which are characterised by concentric 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.

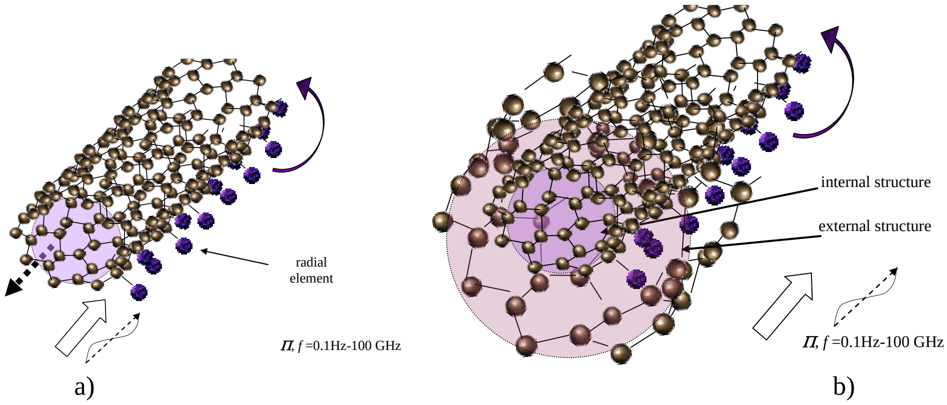

Fig. 1 Geometrical structure of the numerical analysis of surface wave propagation: a) single wire; b) coaxial line.

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 intensities and flux densities:

$$rot\,\boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t} + rot\left(\boldsymbol{v}\times\boldsymbol{B}\right),\quad rot\,\boldsymbol{H} = \boldsymbol{J}_T + \frac{\partial \boldsymbol{D}}{\partial t} + rot\left(\boldsymbol{v}\times\boldsymbol{D}\right),\quad div\,\boldsymbol{B} = \boldsymbol{0},\, div\,\boldsymbol{D} = \rho, \tag{1}$$

where $\boldsymbol{H}$ is the magnetic field intensity, $\boldsymbol{B}$ is the magnetic flux density, $\boldsymbol{J}_\mathrm{T}$ is the total current density, $\boldsymbol{D}$ is the electric flux density, $\boldsymbol{v}$ is the instantaneous velocity of the moving elements, and ρ is the electric charge volume density. Respecting the continuity equation

$$div\,\boldsymbol{J}_T = -\frac{\partial \rho}{\partial t}, \tag{2}$$

the vector functions are expressed by means of the scalar electric potential ϕ_e and the vector magnetic potential $\boldsymbol{A}$, and, after Coulomb calibration, the final relationship between the quantities is expressed as

$$rot\,\boldsymbol{H} = \gamma\left(\boldsymbol{E}+\boldsymbol{v}\times\boldsymbol{B}\right) - \frac{\partial\left(\varepsilon\boldsymbol{E}\right)}{\partial t} + \frac{\gamma}{q}\left(\frac{m_0\left(1-\frac{v^2}{c^2}\right)^{-\frac{1}{2}}\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} + l\,\boldsymbol{v} + k\int_t \boldsymbol{v}\,\mathrm{d}t\right) + \frac{\partial \boldsymbol{D}}{\partial t} + rot\left(\boldsymbol{v}\times\boldsymbol{D}\right) \tag{3}$$

$$m\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} + l\,\boldsymbol{v} + k\int_t \boldsymbol{v}\,\mathrm{d}t = q\left(\boldsymbol{E}+\boldsymbol{v}\times\boldsymbol{B}\right) - \frac{q}{\gamma}\frac{\partial\left(\varepsilon\,\boldsymbol{E}\right)}{\partial t}, \tag{4}$$

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 quantity indexes of the permeabilities μ and permittivities ε r denote the relative quantity value, and 0 denotes the value of the quantity for a vacuum.

Detailed Geometry of the Model of a Periodic Structure

The design of the geometrical model can now be characterized in greater detail. The fundamental element of a graphene-based periodic structure is a benzene core [5]; from the perspective of the stochastic distribution of the instantaneous position and arrangement of C valence electrons, the fundamental element can be schematically described as shown in Fig. 2, [6], Fig. 3.

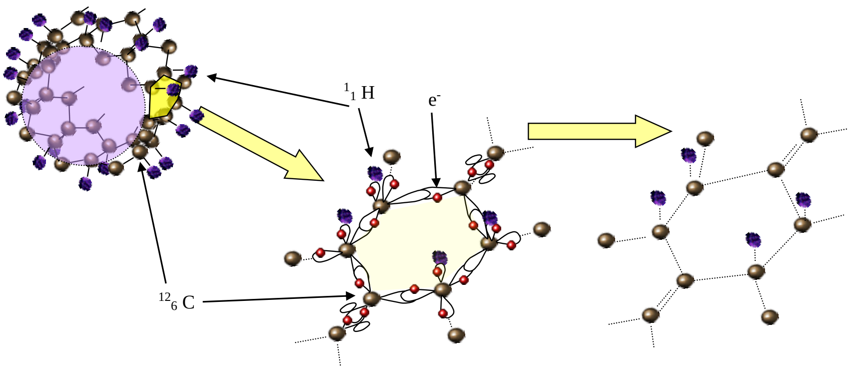

Fig. 2 Geometrical model of the basic structure element with probabilistic distribution of the valence electrons.

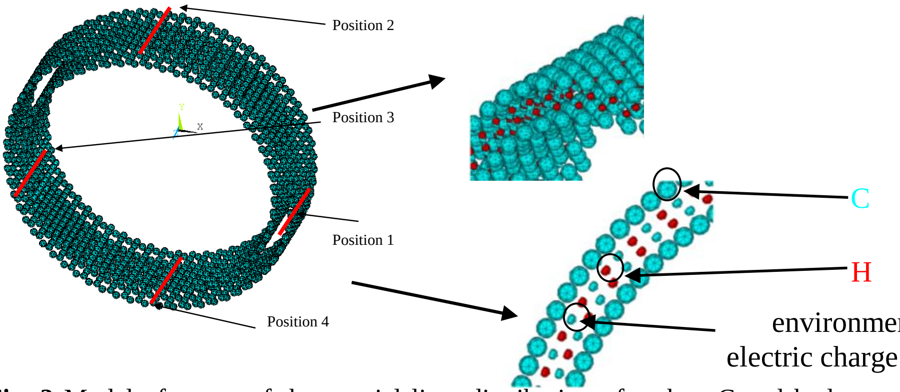

Fig. 3 Model of a part of the coaxial line: distribution of carbon C and hydrogen H atoms in a polymer structrure with a high degree of periodicity.

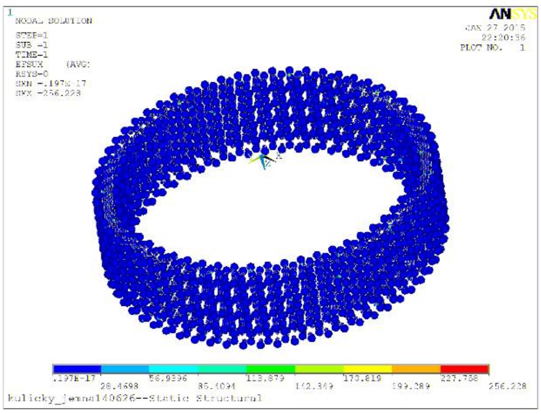

Fig. 4a Distribution of the electric field intensity module: E(t) [V/μm], t_1= 1 ps.

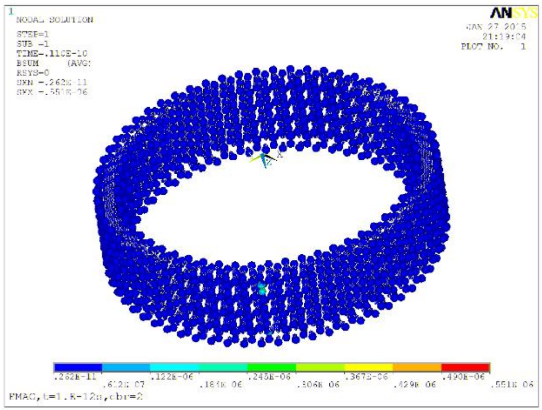

Fig. 4b Distribution of the magnetic flux density module: B(t) [pT], t_1= 1 ps.

Sensor design

The design that includes a coaxial conductor (Fig. 6) exhibiting the diameter of 7nm and external dimensions of less than 1μm must be loaded with suitable impedance at one of its ends, and the entire sensor comprising *N* threads is to be conceived as a Rogowski sensor.

3. Conclusion

We designed a geometrical model of a high periodicity nanostructure, and we also completed a numerical model for the solution and analysis of effects occurring in the propagation of an

EMG wave along the nanostructure. Within the procedure, initial numerical experiments targeting the propagation of an EMG wave in the given nanostructure were carried out too.

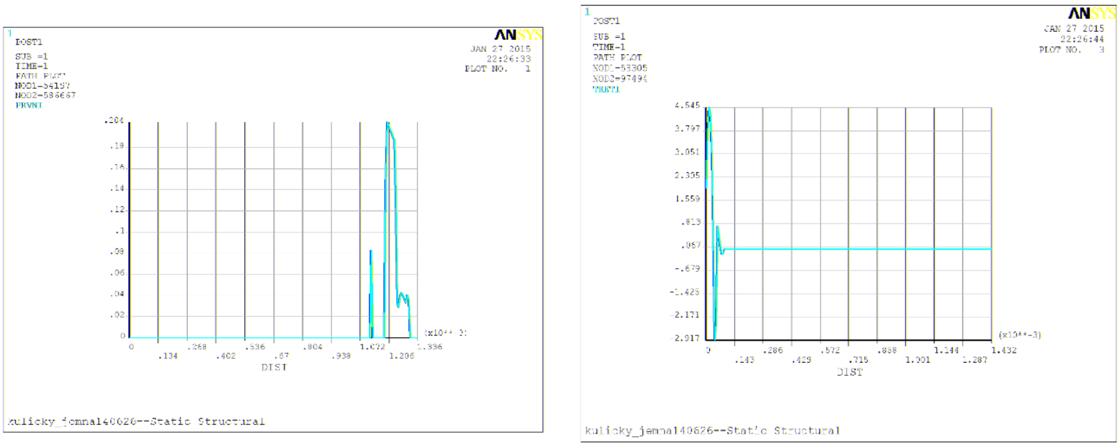

Fig.5 Behaviour of the distribution of the power specific density module $\Pi(t)$ [pW/μm^2], t_1= 1 ps along curve 1, (3).

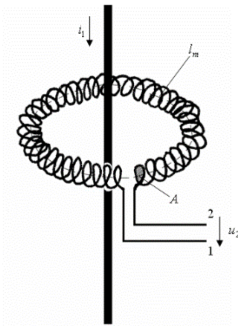

Fig. 6 Design and external dimensions (7nm) of the sensor conceived as a Rogowski sensor.

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