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ORIGINAL PAPER

A meshless approach for electromagnetic simulation of metallic carbon nanotubes

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Abstract In this paper, a study on the electromagnetic behaviour of a single wall carbon nanotube model is described. The electrons available for conduction are treated as a thin cylindrical layer fluid and their motion is described by means of classical hydrodynamics equations in linearized form. These equations are solved in time domain using the Smoothed Particle Hydrodynamics method. The method suitably handled runs on GRID environment.

Keywords Carbon nanotubes · Electromagnetics · Meshless methods · Smoothed Particle Hydrodynamics · GRID computing

1 Introduction

The technological evolution in electronics has become more and more rapid, shrinking the dimension of chips and integrated circuits (IC) and raising the upper frequency limit. In such devices, the traditional conductor materials (copper and noble metals) are no more suitable, due to electromagnetic (EM) phenomena which do not fit with the correct working. The effects of eddy currents and the inducted high-frequency EM fields are the hardest obstacles which limit the development of smaller ICs.

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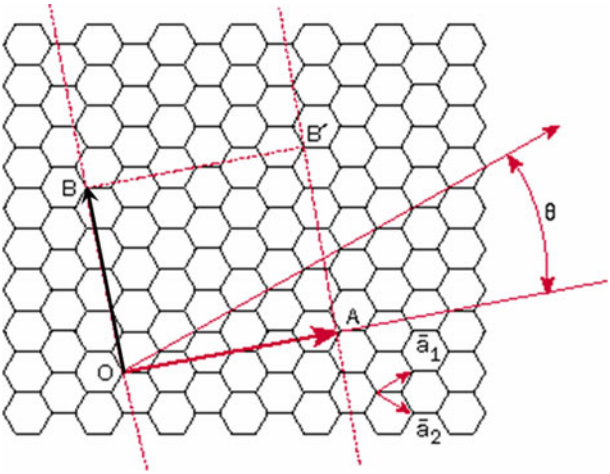

Fig. 1 Graphene sheet. Vectors and geometrical parameters

Today, chip producers are oriented in employing alternative materials for the next generation products. One of the most promising materials is carbon, in form of nanotubes.

Singular Wall Nanotubes (SWNT) and Multi Wall Nanotubes (MWNT) seem to have an optimal behaviour both electromagnetically and thermically. Besides, they have great resilience and low cost when the industrial process for large scale production is optimized.

In the last years, field effect transistor (FET), dipole antennas and interconnects realized by carbon nanotubes have been presented and discussed. The nanotubes have high electrical and thermal conductivity, bear impressive current densities and have good mechanical properties [1,2].

In this paper, the electromagnetic behaviour of carbon nanotubes is investigated assuming the π-electron motion governed by classical equations of dynamics [3,4]. The problem is described by partial differential equations in time domain. The numerical solution is performed by revisiting the Smoothed Particle Hydrodynamics (SPH) method generally used in fluid dynamics context [5]. The proposed formulation is applied to determine the current flowing in a carbon nanotube for different frequencies of the voltage source.

The GRID environment has shown to be suitable to minimize the computational runtime due to the high number of frequencies under investigation.

2 Structure of single wall nanotubes

Carbon nanotubes are obtained rolling bi-dimensional sheets of graphene (an one-atom-thick graphite sheet) along a generic axis [1,2].

In order to effectively describe the nanotube structure, let us consider a graphene sheet (Fig. 1).

The nanotube is described by the vectors $\vec{a}_1$ and $\vec{a}_2$, with $|\vec{a}_1| = |\vec{a}_2| = a_0 = 0.246\,\text{nm}$, forming a 60°angle. The graphene sheet is then rolled with $\mathbf{OA} = n_1\vec{a}_1 + n_2\vec{a}_2$ being the circumference of the tube. This vector, called *chiral vector*, is often described by the pair (n_1, n_2) and denotes univocally the nanotube.

In Fig. 1, $\mathbf{OA} = 4\vec{a}_1 + 2\vec{a}_2$ and the resulting nanotube will be denoted as (4, 2) nanotube.

The *translational vector* **OB**, perpendicular to **OA**, represents the distance after which the surface pattern repeats itself. The rectangle **OABB'** is called *unit cell*.

The properties of the nanotube depend on the angle between the chiral vector and $\vec{a}_1$ (*chiral angle*). Nanotubes with similar diameter but different chiral vectors show totally different behaviours.

In particular, $(n, 0)$ nanotubes are called *zig-zag* nanotubes and show a semi-conductor behaviour, whereas (n, n) nanotube are called *armchair* nanotubes and behave like metallic conductors.

The chiral angle can be expressed as:

$$\theta = \arccos \frac{\vec{a}_1 \cdot \vec{c}}{|\vec{a}_1| \cdot \vec{c}} = \frac{n_1 + n_2/2}{\sqrt{n_1^2 + n_1 n_2 + n_2^2}}, \tag{1}$$

in which $\vec{c} = |\mathbf{OA}| = a_0\sqrt{n_1^2 + n_1 n_2 + n_2^2}$.

This angle is 0° for zig-zag nanotubes and 30° for armchair ones. Both the chiral vector and the chiral angle determine the geometrical parameters of the tube (diameter, number of carbon atoms in the unit cell, length of the translational vector, etc.) as shown in Fig. 2.

The diameter can be expressed as:

$$d = \frac{|\vec{c}|}{\pi} = \frac{a_0}{\pi}\sqrt{n_1^2 + n_1 n_2 + n_2^2} = \frac{a_0}{\pi}\sqrt{N}, \tag{2}$$

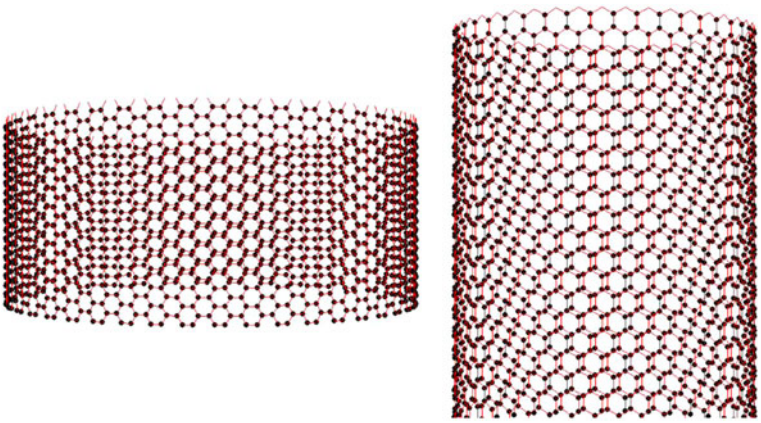

Fig. 2 A (40, 40) nanotube on the left and *a* (40, 0) nanotube on the right

with $N = n_1^2 + n_1 n_2 + n_2^2$.

The translational vector can be expressed as follows:

$$|\mathbf{OB}| = \frac{\sqrt{3N}}{n\Re} a_0, \tag{3}$$

where $\Re = 3$ if $(n_1 - n_2)/3n$ is an integer, otherwise, $\Re = 1$ (n is the greatest common divisor of n_1 and n_2).

Each graphene cell contains 2 carbon atoms and the number of carbon atoms, n_C, in the unit cell can be expressed as the ratio between the lateral area of the nanotube S_L and the area of the singular graphene cell S_g:

$$n_C = 2\frac{S_L}{S_g} = \frac{4N}{n\Re}. \tag{4}$$

3 The model

Studies on the EM behaviour of carbon nanotubes by considering them as transmission lines have been carried out [6]. More recently, a model based on the hydrodynamics of an electron gas has been proposed.

Because of the structure of the carbon-carbon bond in nanotubes, each atom is bonded with other three atoms, thus leaving only an electron available for the conduction (π-electron) [7].

Therefore, the available electrons can be regarded as a single layer electron gas and treated according to the classical motion equations of fluid dynamics [3,4]. Let us consider the classical equations of conservation of density and momentum in linearized form,

$$\frac{\partial \delta n}{\partial t} + n_0 \nabla_{||} \cdot \vec{v} = 0 \tag{5}$$

$$n_0 \frac{\partial \vec{v}}{\partial t} = -\frac{1}{m_{eff}} \nabla_{||} \delta p - e\frac{n_0}{m_{eff}} \vec{e}_{||} - \frac{1}{\tau} n_0 \vec{v}, \tag{6}$$

being n_0 the density number of electrons able to conduct at the equilibrium, $\vec{v}$ the speed of the electrons, p the pressure due to the fluid motion, e and m_{eff} the electron charge and effective mass, $\vec{e}$ is the electric field directed along the tube axis and τ is the relaxation time, respectively. The symbol $_{||}$ refers to the direction of the tube axis.

By expressing the pressure as

$$\delta p = \left(\frac{\partial p}{\partial n}\right)_{n=n_0} \cdot \delta n = m_{eff} c_S^2 \cdot \delta n, \tag{7}$$

in which c_S is the thermodynamic speed of sound in the electron fluid, and by expressing the current and superficial charge densities on the lateral surface of the nanotube

as

$$\begin{aligned} \sigma &= -e\delta n\left(\vec{r}_S, t\right), \\ \vec{j} &= -en_0\vec{v}\left(\vec{r}_S, t\right) \end{aligned} \tag{8}$$

in which $\vec{r}_S$ is a vector identifying a generical point on the lateral surface of the tube, the Eqs. (5) and (6) become:

$$\frac{\partial\sigma}{\partial t} + \nabla_{||} \cdot \vec{j} = 0 \tag{9}$$

and

$$\frac{\partial \vec{j}}{\partial t} + \frac{1}{\tau}\vec{j} + c_S^2\nabla_{||}\sigma = e^2\frac{n_0}{m_{eff}}\vec{e}_{||}. \tag{10}$$

These equations hold only for tubes with $n_1, n_2 < 50$ and with axial length greater than the tube diameter.

The values for the parameters c_S, τ and $\frac{n_0}{m_{eff}}$ are detailed in [7].

4 The numerical approach

To solve both equations in time domain, the *Smoothed Particle Hydrodynamics* (SPH) method is used. The SPH method is a powerful instrument for investigating the motion of fluids and gases. It is a meshless method since it does not require a computational grid with fixed nodes [5]. The problem domain is discretized by means of "particles" and the function values and their derivatives for each particle are evaluated by using the information of "near" particles (Fig. 3).

Namely, the integral approximation of a function $f(x)$ is

$$\langle f(\vec{x})\rangle = \int_\Omega f(\vec{x}')W(\vec{x} - \vec{x}', h)d\vec{x}', \tag{11}$$

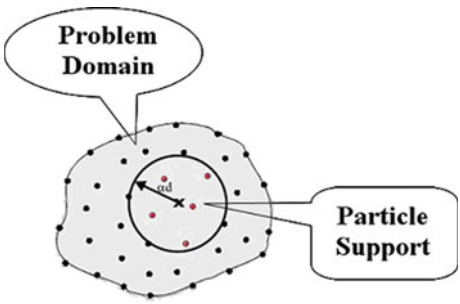

Fig. 3 Problem domain and particle support

where $W(\vec{x} - \vec{x}', h)$ is a suitable kernel function, defined only in the particle support, Ω is the problem domain, h is the smoothing length and $\vec{x}$, $\vec{x}'$ are the position vectors of the particles.

The SPH method is used to approximate the spatial derivatives of Eqs. (9) and (10) [8]. The time derivatives are evaluated with a finite difference scheme.

In the simulation, the cubic B-Spline presented in [5] is used. The nanotube is discretized by 4,000 particles, each accounting for 8 electrons scattered on the nanotube surface. Each particle is located in the center of mass of the 8-electron group.

A unitary voltage source at different frequencies is applied and the current response is measured.

The simulations at different frequencies run on GRID environment by means of the Message Passing Interface (MPI) paradigm.

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