A CONTINUAL APPROACH TO VAN DER WAALS INTERACTIONS IN CARBON NANOTUBE BASED SYSTEMS

Y. Belahurau, V. Barkaline
Belarusian National Technical University, Minsk, Belarus

Abstract – Ordered arrays of carbon nanotubes (CNT) are promising elements of nanoelectromechanical systems based on transformation of electromagnetic fields into mechanical motion. Simulation of these phenomena accounting various nonlinear interactions can be realized on the basis of macroelectrodynamics of moving media, theory of elasticity and van der Waals interactions' phenomenological theory. The balance equations of mass, momentum, angular momentum and energy as well as entropy inequality describing interacting continua of the mass, electric charge and internal spin are presented. To include van der Waals forces the additional terms are introduced into these equations which transform the system into indegro-differencial one. It is shown that integral terms can be neglected if the gap between tubes is greater than CNT outer diameter. The occurrence of multiple resonant vibrations of ordered CNT arrays is characteristic of them. Solving the system numerically the essential influence of van der Waals forces on CNT array resonant frequencies was proved.

I. INTRODUCTION

Dynamic mechanical behaviors of CNTs have been studied widely in recent years. Ordered arrays of carbon nanotubes (CNT) are prospect materials of nanoelectromechanical systems based on transformation of electromagnetic fields to the mechanical motion [1]. Such arrays may be used as sensitive elements of different sensors with acoustoelectronic output signal [2]. Electromechanical coupling theory for such arrays is based on combined solution of kinetic equation for electrons, Maxwell's equations and the equations of lattice dynamics [3]. But there can be also a phenomenological approach based on macroscopic electrodynamics and continuum mechanics. Correct simulation of electromagnetic and mechanical behavior of such system requires accounting of all interactions in the system as precise as possible. An approach [4] can be used here. In this article we tried to take into account van der Waals's interactions in CNT arrays and analyze the influence of these interactions on the mechanical resonance dynamics of CNT arrays.

II. FUNDAMENTAL OF THE PROBLEM

Development and creation of the continual approach which can take into account van der Walls' (vdW') interactions is the main aim of the article. VdW' interactions is described with the through the Lennard–Jones (LJ) potential [5].

$$U(\vec{r}) = -\frac{C_6}{\vec{r}^{\,6}} + \frac{r_0^6 \cdot C_6}{2 \cdot \vec{r}^{\,12}}, \tag{1}$$

where r_0=3.88 A, $c_6=2.5\cdot10^{-77}$ J·m^6.

Volume force density acting on tube t_1 of array is represented as:

$$\vec{F}(\vec{r}) = 6 \cdot C_6 \cdot r_0^{-7} \cdot \frac{\vec{r}}{r_0} \cdot \left(\frac{r_0}{\vec{r}}\right)^8 \cdot \left(\left(\frac{r_0}{r}\right)^6 - 1\right). \tag{2}$$

Modelling interaction of nanotubes {10, 10}, length is 100 A, outer diameter is 13.56 A, internal diameter 3.354 A, density is 2260 kg/m^3 , atom concentration $n=2{,}7587\cdot10^{29}$ m^{-3} have been performed for studying van der Waals' interactions influence on resonance frequencies of CNT arrays. Elasticity modulus of CNT has been calculated with a molecular dynamics approach (force field is MM+): $c_{11} = c_{12}= 44{,}6\cdot10^{10}$ Pa, $c_{12}=14{,}2\cdot10^{10}$ Pa, $c_{13} = c_{23} =13{,}9\cdot10^{10}$ Pa, $c_{33}=119\cdot10^{10}$ Pa, $c_{44} = c_{55}=$

$22{,}6 \cdot 10^{10}$ Pa, c_{66}=$14{,}9 \cdot 10^{10}$ Pa. Minimal distance between nanotubes is 3.4 A, 6 A, 10 A. In figure 1 the tubes are demonstrated with using finite element mesh.

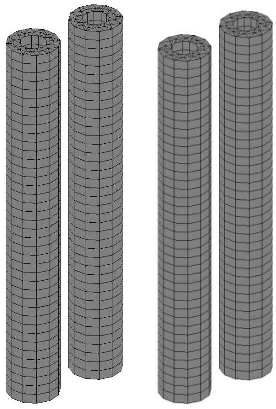
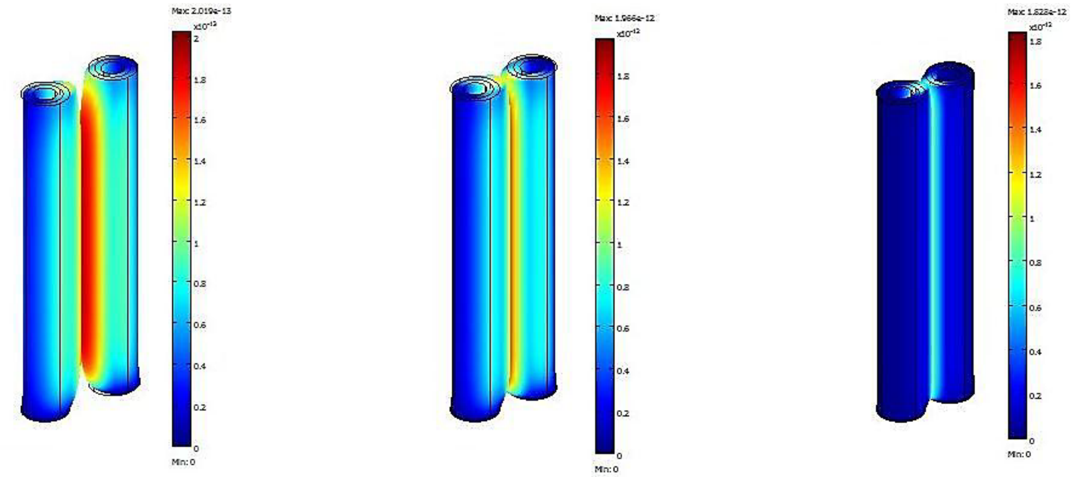


Figure 1 – Nanotubes with using finite element mesh

III. Van der Waals' interactions' influence on CNT array eigenfrequencies

In figure 2 the results of modeling of CNT static displacement in consequence of van der Waals' interactions are presented.



a) b) c)

Figure 2 – CNT static displacement as consequence of van der Walls' interactions:
a) distance between CNT is 10 A; б) 6 A: в) 3,4 A

Eigenfrequencies have been calculated for the nanotubes which have been deformed in consequence of van der Waals' interactions. The results are presented in table 1.

TABLE 1 – The CNT array resonance frequencies dependence on distance between nanotubes

Mode shape	Frequencies, GHz			
	Distance between the nanotubes			
	∞	**10 A**	**6A**	**3.4 A**
The 1st bend sagittal on the right tube	43,6112	41,39366	8,538689	16,02657
The 1st bend sagittal on the left tube	43,6112	41,3937	8,544155	16,02649
The 1st bend normal on the right tube	44,4347	41,66737	11,7175	21,07665
The 1st bend normal on the left tube	44,4347	41,66789	11,7232	21,19131
The 1st inflating on the right tube	213,9189	205,8242	58,15274	59,22345
The 1st inflating on the left tube	213,9189	205,8243	58,15945	59,24583
The 2d bend sagittal on the right tube	227,6754	217,2999	84,75225	87,56229
The 2d bend sagittal on the left tube	227,6754	217,301	84,75846	87,58248
The 2d bend normal on the right tube	234,8002	236,6432	112,2834	116,2563
The 2d bend normal on the left tube	234,8002	236,644	112,3166	116,6587

IV. CONCLUSION

Modeling the dynamics of CNT arrays taking into account nonlinear effects can be performed with the help of continuous electrodynamics of moving bodies, the elasticity theory and van der Waals' interactions' theory. Accounting of van der Waals' interactions transforms a set of balance equations to an integro-differential one. If distance between nanotubes in an array is more than tube outer diameter the integral terms may be neglected. Influence of van der Waals' forces is considerable if distance between nanotubes in the array is 3–10 A.

REFERENCES

[1] V. Barkaline, I. Abramov, E. Belogurov, A. Chashynski, V. Labunov, A. Pletezhov and Y. Shukevich, Nonlinear Phenomena in Complex Systems 15, 23 (2012).

[2] V. Barkaline and A. Chashynski, in Chemical Sensors: Comprehensive Sensor Technologies, V. 7, DOI: 10.5643/9781606503171/ch7.

[3] V. M. Kontorovich, Physics Uspekhi 142, 265 (1984).

[4] J. Mozhen. Electromagnetic continuum mechanics. M: Mir, 1991. 560 p.

[5] Lennard-Jones, J.E., 1931. Cohesion. Proceedings of the Physical Society 43, 461–482.