MOLECULAR DYNAMICS SIMULATION OF CARBON NANOTUBE ARRAYS RESPONSES ON MECHANICAL AND ELECTRICAL HIGH FREQUENCY FORCES

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Abstract – Torsional mode excitation of carbon nanotube bundle in high frequency electric field is revealed by molecular dynamics numerical experiment. Signal propagation in linear chain of carbon nanotubes linked by van der Waals forces is discussed.

I. INTRODUCTION

Study of carbon nanotube bundles behavior in electromagnetic field is of essential interest in the design of nanodevices of radio and UHF frequency regions [1]. This interest is caused by the existence of resonant properties of carbon nanotubes (CNT) and significance of van der Waals interactions in determining of the dynamics of CNT arrays, which lead to strong nonlinearity in their behavior in electromagnetic and acoustic fields.

The most applicable method of simulation of CNT based nanosystems seems to be the method of molecular dynamics, which implies the calculation of trajectories of all atoms of the systems by numerical integration of classical equations of motion with empirically defined force fields describing interatomic interactions [2].

II. EXCITATION OF CNT BUNDLES BY HIGH FREQUENCY ELECTRIC FIELD

In the presented paper we used the molecular dynamics package NAMD (NAnoscale Molecular Dynamics) [3] with graphical interface VMD (Visual Molecular Dynamics) [4], which are freely available. NAMD package uses the CHARMM force field developed mainly for the description of intermolecular interactions in biopolymers. Its usage for CNT array modeling seems to be proved too.
The system under study was the array of seven parallel nanotubes cupped from one side with length 200 Å and diameter 13 Å with chirality parameters {10,10}. CNTs formed regular triangle lattice with minimal intertube distance 6 Å (Figure 1, initial state picture). Nanotube cups can have manually introduced electrical charges, which are totally compensated by opposite charges at graphene layer placed under the array. Harmonically varying charges on the array and graphene layer simulated the external electric field with frequency 25 GHz. Simulation results for several times are presented in Figure 1 too. Total simulation time was 41 ps.

The data presented show the excitation of binding modes as well as torsional mode of CNT bundle. The last observation seems to be new and unexpected. Besides that the small amplitude vertical motion of CNT was observed with frequency much more high then frequency of charging which corresponds to the excitation of vibrational eigen mode of traction-and-compression type.

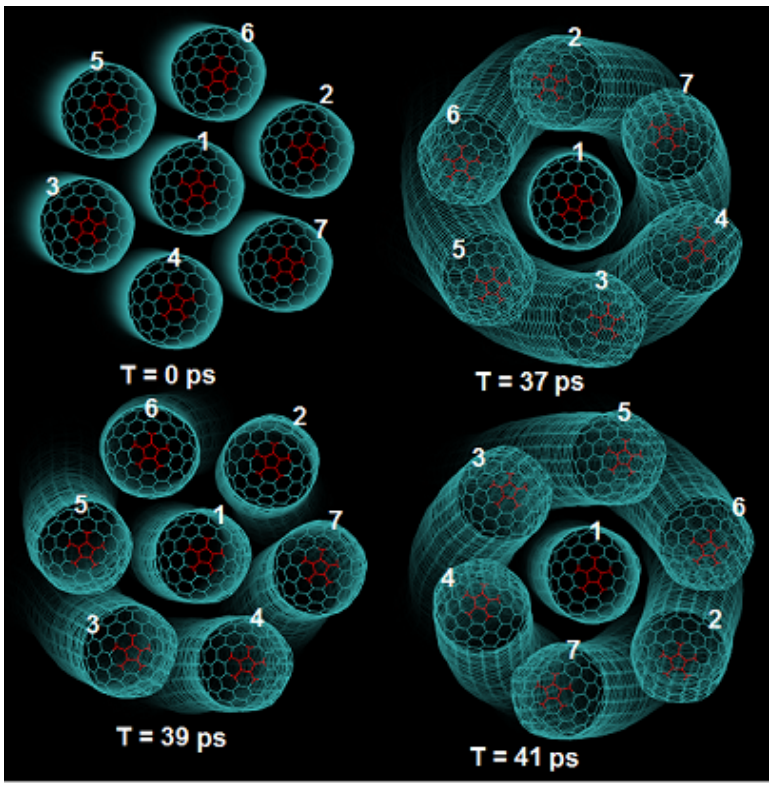

Figure 1 – Torsional mode of CNT bundle under the action of an electrical field

III. PROPAGATION OF EXCITATION IN CNT LINEAR CHAIN

In Figure 2 the results of simulation of the mechanical excitation of CNT linear chain are presented. The system under study was the array of seven one-side cupped nanotubes with length 200 Å, diameter 13 Å and chirality parameters {10,10}. Before geometry optimization parallel CNTs formed linear chain with minimal intertube distance 14 Å. After such optimization one get the array configuration presented at the first picture in Figure 2. Total simulation time was 100 ps.

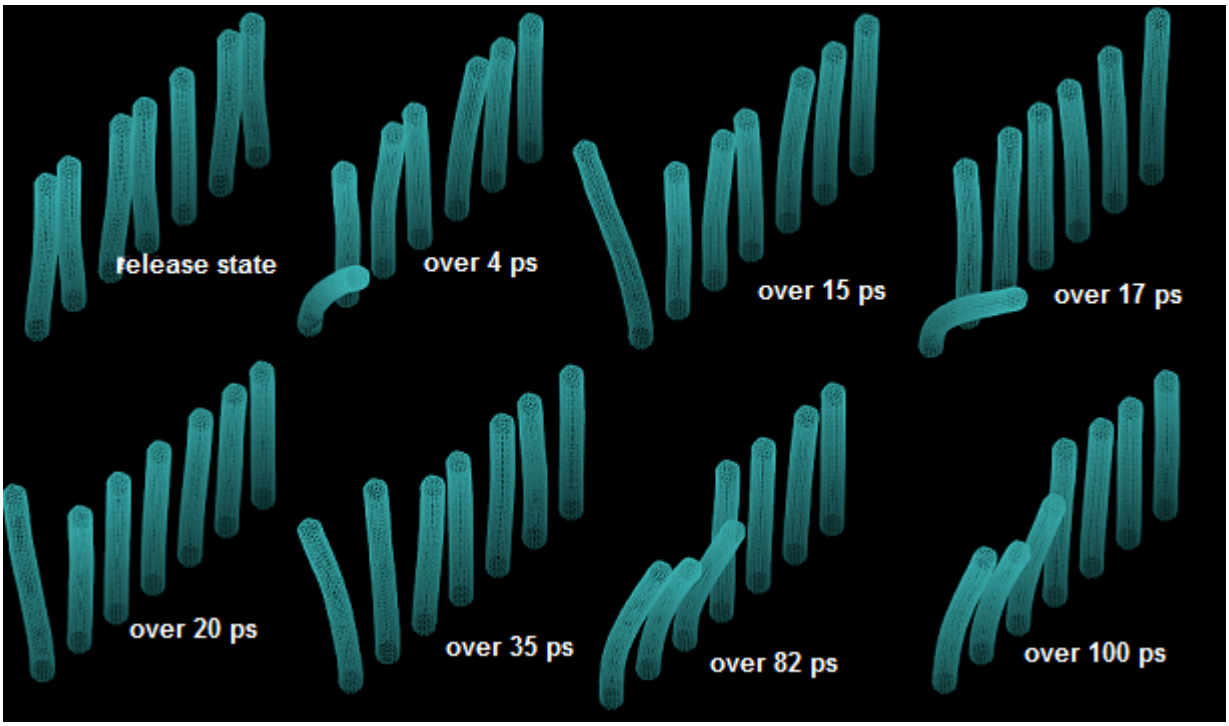

Figure 2 – CNT chain excited by giving the velocities
to the atoms on the cup of first tube in transversal direction

The idea of numerical experiment was the mechanical excitation of the array by giving transversal velocity to the atoms of the cup of first tube and observing the propagation of excitation through the chain due to van der Waals interaction. Finite state of the array is interpreted as the effect of input signal. Varying the signal one gets various output state of the array. In principle, such array plays a role of analogous memory nanodevice.

It is necessary to note that displacement amplitude of the tubes decreases with the distance along the chain and for fifth, sixth and seventh tubes the displacements have not component clearly corresponding to the input signal. The response to the signal does not propagate further forth tube. Additional studies are needed for clarification this damping and memory effect. In principle such linear array could be used as learning element of nanosize artificial neuronal network.

IV. Conclusion

Numerical experiments on the electrical and mechanical excitation of carbon nanotube arrays of various form are realized with the NAMD+VMD simulation packages. For CNT bundle in high frequency electric field the excitation of torsional mode is discovered. For CNT linear chain array the damping of the mechanical excitation is found and boundary memory effect is described.

References

[1] Barkaline V., Abramov I., Belogurov E., Chashynski A., Labunov V., Pletezhov A., Shukevich Y. Simulation of Carbon Nanotubes and Resonant Excitation of Their Mechanical Vibrations of by Electromagnetic Field for Nanoradio Applications / V. Barkaline [et al.] // Nonlinear phenomena in complex systems, vol. 15, no. 1 (2012), pp. 23 – 42.

[2] Frenkel D., Smit B. Understanding Molecular Simulation. From Algorithms to Applications – London: Academic Press, 2002, 638 p.

[3] Phillips, J.C. Scalable molecular dynamics with NAMD / R. Braun, W. Wang, J. Gumbart, E. Tajkhorshid, E. Villa. C. Chipot, R.D. Skeel, L. Kale, K. Schulten. // J. Comp. Chem, 2005. P. 1781 – 1802.

[4] Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics", J. Molec. Graphics, 1996, vol. 14, pp. 33-38.