

PLASMA-MECHANICAL OSCILLATIONS IN CARBON NANOTUBES ARRAY

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Abstract. The results of the simulation of plasma-mechanical oscillations in carbon multiwalled nanotubes array under electromagnetic radiation are presented considering thermal fluctuations, internal stress, static load and the ponderomotive forces between the nanotubes.

1. Introduction

Recently a great interest in the study of the interaction between the electromagnetic radiation (EMR) with the frequency range from 1 GHz to 1 THz and the carbon nanotubes (CNTs) arrays has grown up. Despite the large number of existing works on measurements and modeling of these processes, many data still remain unclear. The cases of interaction of the EMR with individual single-walled CNTs are mainly considered in the theoretical works, while the known phenomenological models developed for composites containing nanoparticles are used in the experimental works for the interpretation of the data obtained.

The real arrays of aligned CNTs are far from perfect; they are characterized by heterogeneity, the presence of branches, intersections, curves, bridges, contacts between the tubes and the inclusion of magnetic nanoparticles. The characteristic dimensions of the free fragments of CNTs between the points of attachment, contact, or bending are tens or hundreds of nanometers.

Free fragments of CNTs in the array, having high elasticity, undergo mechanical vibrations. Such fluctuations are caused both by external (mechanical stress, heat, electric and magnetic fields, currents) and inner (thermal fluctuations, magnetoelastic effects, residual strains and stresses) factors. The free CNT fragments are characterized by natural frequencies of mechanical oscillations, the values of which are determined, additionally to the CNTs radii, the elastic moduli and the lengths of these areas, by the presence of fixtures and strains.

The aim of the work is to simulate the plasma-mechanical oscillations in a multi-walled carbon nanotubes array under the influence of electromagnetic radiation taking into account the ponderomotive forces between the nanotubes, thermal fluctuations, stress and static load.

2. Plasma-mechanical oscillations

The equation of mechanical oscillations of the free CNT fragment of the length L , fixed on two sides, being under the influence of thermal fluctuations, accidental loads and the ponderomotive force can be written as [1]:

$$\frac{\partial^2 w}{\partial t^2} + \gamma \frac{\partial w}{\partial t} + \beta \frac{\partial^4 w}{\partial z^4} = F(z, t), \quad (1)$$

where w is the deviation of vibrating nanotube from equilibrium, γ is the damping factor of

the mechanical system. Here γ is a constant that determines the damping coefficient $\beta = J / M$, where M is the mass of the nanotube per unit length, J is its bending stiffness, $F(z, t)$ is the force per unit length normalized to the mass M .

By the substitution $w(z, t) = \exp[-(1/2)\gamma t]u(z, t)$ equation (1) is transformed to

$$\frac{\partial^2 u}{\partial t^2} + \beta \frac{\partial^4 u}{\partial z^4} - \frac{1}{4} \gamma^2 u = \exp(\gamma t / 2) F(z, t). \quad (2)$$

Consider the solution of (2) in the region $0 \leq z \leq L$ with the initial conditions in a general form $u(z, 0) = u_0(z)$, $\partial u(z, t) / \partial t = g(z)$ at $t=0$. The solution is represented by Green's function $G(z, \xi, t)$ [2]:

$$\begin{aligned} u(z, t) = & \frac{\partial}{\partial t} \int_0^L u_0(\xi) G(z, \xi, t) d\xi + \int_0^L g(\xi) G(z, \xi, t) d\xi + \\ & + \int_0^t \int_0^L \exp(\gamma \tau / 2) F(\xi, \tau) G(z, \xi, t - \tau) d\xi d\tau. \end{aligned} \quad (3)$$

In this paper, the position CNT is static for initial conditions, some static bending presents, but there is no CNT vibrations and therefore $g(\xi) = 0$.

For the case where the boundaries defined by a function and its first derivative: $u=0$, $du/dz=0$ at $z=0, L$, the Green's function after the transformations is written as:

$$G(z, \xi, t) = \frac{1}{L} \sum_{n=1}^{\infty} \frac{\phi_n(z) \phi_n(\xi) \sin(t \omega_n)}{[\cosh[(2n+1)\pi / 2]]^2 \omega_n}, \quad (4)$$

where $\omega_n = \sqrt{(\beta / L^4)[(2n+1)\pi / 2]^4 - (1/4)\gamma^2}$ are the characteristic vibration frequencies, the function

$$\begin{aligned} \phi_n(\eta) = & [\sinh[(n+1/2)\pi] - (-1)^n] \cdot \\ & [\cosh[(n+1/2)\pi\eta] - \cos[(n+1/2)\pi\eta]] - \\ & - \cosh[(n+1/2)\pi] \cdot [\sinh[(n+1/2)\pi\eta] - \sin[(n+1/2)\pi\eta]], \end{aligned} \quad (5)$$

where $\eta = z(\xi) / L$.

Let us define the force F . If CNTs are close to each other (when the spacing between them $s < L$), a distributed repulsive force between them in the presence of distributed charge $\rho(z, t) / 2$ at each of them, it is $F = \rho^2(z, t) / 2s\epsilon_0 M$ (there is no self-consistent plasma and mechanical vibrations at this stage). If the quality factor of the main resonance of plasma oscillations is sufficiently high, the external signal spectrum is rather narrow near the resonant frequency of the plasma oscillations of the force per unit length $F(z, t)$ can be written as follows [3]:

$$F(z, t) = [\rho_0^2(t) / 2s\epsilon_0] \sin^2(k_m z) / M, \quad (6)$$

where $\rho_0(t)$ is the value of the linear charge density at some CNT's point, the wave number

$k_m = (\pi/L)(2m+1)$ characterizes the charge distribution along the CNT's length.

Due to the presence of noise process the force will be written as $F(z, t) = [\rho_0^2(t)/2s\epsilon_0]\sin^2(k_m z)/M + \sigma\zeta(t)$, where σ is the parameter, which is the amplitude of the noise process, $\zeta(t)$ is a random value in the $[-1, 1]$ interval, which varies with discrete time step, acting as a time correlation. For white noise: $\langle \zeta(t)\zeta(t') \rangle = \delta(t - t')$.

The fluctuations of charge $\rho_0(t)$ are determined by the characteristic frequencies of plasma oscillations, which are excited both by passing a current through a nanotube, and external radiation. EMR generates eddy currents in the conductive CNTs with characteristic frequencies that depend on the CNTs size, their conductivity and the Fermi velocity. The frequencies values are between 50 GHz and above.

3. Results and discussion

Multi-walled CNTs with a diameter of 30-50 nm and a length of 300-500 nm oscillate with a natural frequency of the mechanical vibrations of 2.1 GHz and have a quality factor of 1000 at room temperature. The resonant frequency of the mechanical vibrations is $f_s = v[(d_{out}^2 - d_{in}^2)(E/\rho)^{1/2}/8\pi L^2]$, where the constant $v = 1.875$ for the fundamental frequency, 4.694 - for the second harmonic. For the CNTs segment with $d_{out} = 55$ nm, $d_{in} = 10$ nm and a length of 350 nm and modulus $E \sim 10^{12}$ Pa, the resonance frequency $f_s \sim 1$ GHz [3]. The ratio of the linear bending stiffness to CNTs weight $\beta/L^4 = (12\pi \cdot E/160L^3)(d_{out}^4 - d_{in}^4)/M$, attenuation coefficient $\gamma = 2\pi \cdot f_{res}/Q$. For the CNT with the mass $M = 1.5 \cdot 10^{-18}$ kg, $\sqrt{\beta/L^4} \sim 1$ GHz.

The action of a mechanical static load is taken into account by the introduction of the initial bending of the CNT $u_0(z) \sim \sin(\pi z)$, depending on location, but not on time. The calculations performed have shown that the mechanical vibrations of the CNT (in the presence of initial bending of CNTs under static load) can be excited:

- Under the influence of external electromagnetic radiation,
- Due to the charge fluctuations of neighboring CNTs by an external electromagnetic radiation corresponding to their resonant frequency (neighboring CNTs vary in size and characteristics from the original CNT).

In the absence of an external force F the oscillations are damped with a characteristic time determined by the damping constant γ . In other cases, the oscillations are forced.

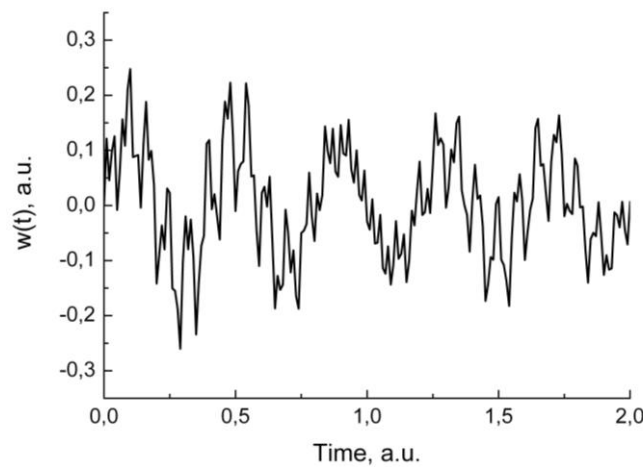


Fig. 1. CNT fluctuations in the case of relatively small external force:

$$u_0(1/2)\omega_1 > \langle F(1/2, t) \rangle.$$

We consider the presence of the initial bending of CNTs and an external force (such as due to EMR exposure on CNT, and due to the charge oscillations of the neighboring CNTs). The results obtained for the case of a relatively small external force are shown in Fig. 1 for center of CNT corresponding to the center of the free CNT fragment. It is found that the oscillations are characterized by damping and higher harmonics.

With the growth of the external harmonic force with the frequency of about from 100 to 200 GHz, the CNTs oscillations are amplitude-modulated variations with the two specific frequencies (Fig. 2). The analysis of the spectra shows that they are quasi-periodic. To simulate the effect of noise processes the normal distribution of the random variables has been used (Fig. 3). The preliminary results of calculations have shown the presence of the noise component of force to lead to noise oscillations and their transition into stochastic ones.

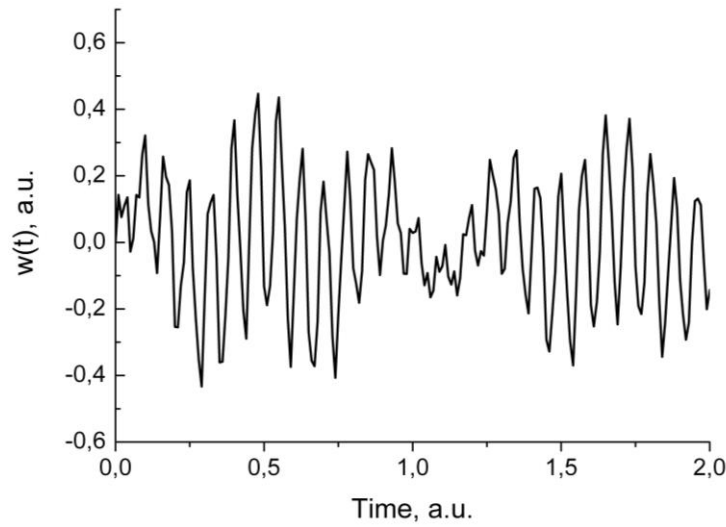


Fig. 2. CNT fluctuations in the case of relatively large external force: $u_0(1/2)\omega_1 < \langle F(1/2, t) \rangle$.

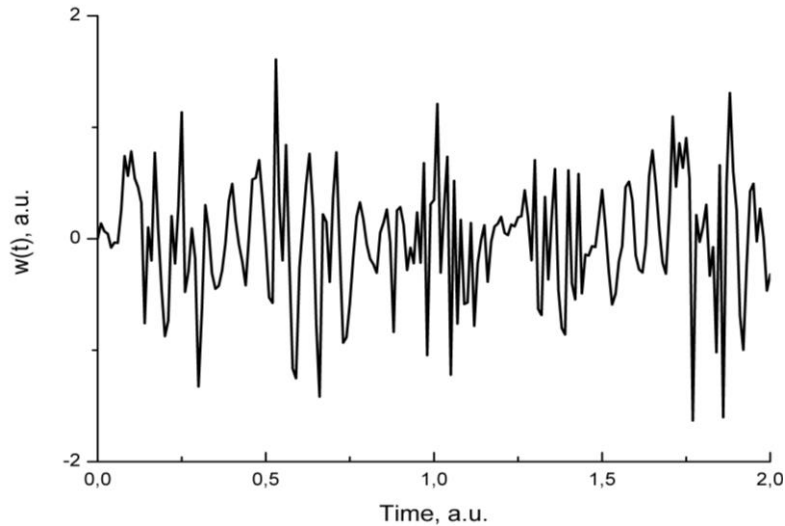


Fig. 3. CNT fluctuations in the case of relatively large external force and significant noise: $u_0(1/2)\omega_1 < \langle F(1/2, t) \rangle$.

4. Conclusion

The calculations of plasma-mechanical oscillations of the CNTs have been performed by using the developed model, which takes into account the initial bend, the effect of

electromagnetic radiation on the CNTs, the charge fluctuations in the neighboring CNTs and the presence of the noise component. The regularities of the mechanical oscillations of CNTs, caused by the charge redistribution in CNTs under the influence of electromagnetic radiation, the initial static bend of CNT and noise, have been established.

It is shown, that in the case of a small external force as compared with the influence of the initial bend, the mechanical oscillations of CNTs are characterized by attenuation. For the case of a relatively large external force in comparison with the influence of the initial bend, the mechanical oscillations are quasiperiodic, amplitude modulated, with the two specific frequencies. For the case of relatively large external force and the significant contribution of noise component, the mechanical oscillations turn into stochastic ones.

References

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