A THz-band Emitter Based on a Single-Walled Carbon Nanotube with Encapsulated Fullerenes

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***Abstract* — We propose a theoretical model for a THz-band emitter based on a carbon nanopeapod formed by a nanotube (10,10) with three encapsulated fullerenes C_{60}. The radiating element is the free charged fullerene C_{60}, which rapidly oscillates in a potential well created by the atomic framework of the nanotube and several uncharged fullerenes polymerized with the tube, as well as with each other. Motion of the charged fullerene and the radiation frequency can be controlled using an external electric field. It was found that stable THz radiation with the frequency of 0.36 THz could be realized at 300 K in the dc electric field of 10 V/m.**

I. Introduction

One of the actual problems of modern applied physics is the exploration of the terahertz frequency range. The interest to this range is due to the broad application prospects of terahertz radiation in both basic and applied research, as well as in various technological areas. Most existing sources of terahertz radiation developed up to date are either bulky (gyrotrons, free-electron lasers) or low-power. The use of carbon nanostructures would solve the both indicated problems. There already exist works devoted to the development of miniature electron current sources for vacuum THz-band devices [1] and sources of THz radiation based on carbon nanotube (CNT) arrays [2]. However, the problem of creating a THz radiation source operating on a single nanotube has not been solved yet. By now, there are no theoretical models and prototypes of such nano-emitters. In this paper, we propose a new model of the terahertz emitter based on a single-walled CNT with encapsulated fullerene molecules [3].

II. Results

Schematic illustration of the proposed device is shown in Fig. 1. The physical principle of the nano-emitter operation is based on oscillation of the charged fullerene C_{60} in the potential well inside the armchair nanotube with chiral indices (10,10). The potential well is created by the van der Waals attraction of the free fullerene by the tube walls and by three uncharged fullerenes C_{60}, which are chemically bonded with each other and with atoms of the tube from the inside. Such a compound ensures the stability of the formed potential well for the free fullerene C_{60}. Atomic structure of the nanotube with the encapsulated fullerenes and the behavior of the free fullerene inside the potential well are investigated by the MDTB method [4] using the original software package KVAZAR [5].

We consider free motion of the molecule C_{60} induced by the thermal fluctuations, as well as the motion of the pre-charged fullerene C_{60}^+ under the influence of an external electric field. The simulation reveals that the free oscillation of the fullerene C_{60} at 300 K is irregular and is characterized by an average frequency ~ 0.3 THz. Irregularity in the fullerene oscillations is caused by a complex nature of the molecule motion. Besides the translational motion, rotation also takes place during the oscillations. As a result, the energy is spent for turns and rotations of the fullerene, which lead to its braking.

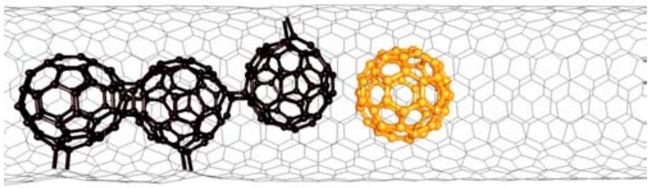

Fig. 1. Model of the nano-emitter: configuration of the fullerenes inside the carbon nanotube with chiral indices (10,10).

To stabilize the fullerene oscillations we propose using an external electric field. Initially, we consider the oscillations of the charged molecule C_{60}^+ in the electric field with the strength of 1 V/μm along the CNT axis. As a result, the character of the C_{60}^+ motion changes significantly. First, the entire trajectory is shifted to the region of positive CNT axis. Second, the irregularity of the periodic motion is increased. Thus, the dc electric field with strength of 1 V/μm does not lead to regular oscillations of the charged fullerene.

In order to examine this phenomenon, we calculate the temporal dependence of temperature for the oscillating fullerene. The calculations reveal that the initial temperature of 300 K is not maintained constant during the oscillation process. The temperature varies with the amplitude of 20 K. In addition, the temperature decreases during the oscillation. This argues occurrence of the energy losses in the system. The losses occur due to the radiation produced by an accelerated motion of the charged fullerene as well ae due to the energy transmitted to environment. To specify the temperature effect on the oscillation process we carried out a series of numerical simulations. Within these simulations, free oscillations of the fullerene and oscillations under an external electric field were studied at the temperature of 50 K.

The character of the fullerene oscillation changes at low temperatures. It becomes regular because the fullerene rotation does not occur during the motion. The analysis of the temperature variations during the oscillation shows that the temperature varies within 46-52 K. The frequency of the fullerene oscillations decreases to 91 GHz at 50 K. At the same time, the external electric field has almost no effect on oscillations.

Thus, from the results of numerical simulations at $T = 50$ and 300 K one can conclude that the thermal motion of C_{60} determines the nature of oscillations in the potential well and

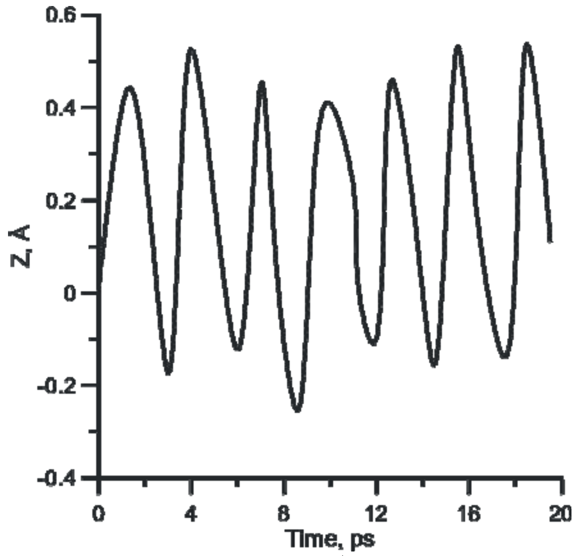

Fig. 2. Position of the mass center for C_{60}^{+} oscillating in the potential well under the external field with the strength of 10 V/μm [3].

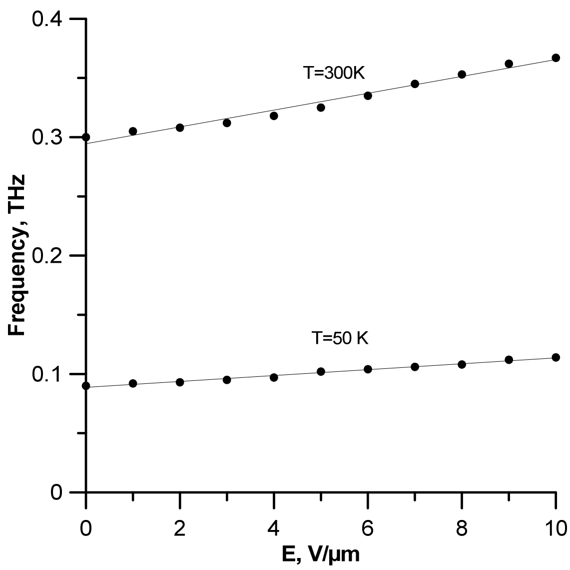

Fig. 3. Oscillation frequency versus intensity of the electric field strength [3]

the proper oscillations frequency. The electric field with strength of 1 V/μm does not cause any specific oscillations and does not affect their frequency.

At the next stage, we perform numerical simulation at $T = 300$ K and at different values of the electric field strength in the range of 1-10 V/μm. Periodic oscillation of the C_{60}^{+} in the potential well is observed at the field strength of ~10 V/μm, as shown in Fig. 2. At such value the field strength, the oscillation amplitude is equal to 0.065 nm and the oscillation frequency is 0.36 THz.

The radiation efficiency of the considered nanoemitter in the terahertz range at the temperature of 300 K under electric field with strength of 10 V/μm was calculated to be 12%. This value was obtained as the ratio of the radiating power to the power imparted to the fullerene by the electric field [6].

The dependence of the oscillation frequency at 50 K and 300 K on the electric field strength is presented in Fig. 3. The frequency linearly grows with the electric field.

III. Summary

Thus, we propose a new model for a THz emitter based on the single-walled carbon nanotube with encapsulated fullerenes (a carbon nanopeapod). The operation principle of the device is based on oscillation of the charged fullerene C_{60} inside the nanotube in the constant electric field. It does not require a dc magnetic field or an RF-field.

The numerical simulations show that the operation of the nanoemitter is mainly determined by external conditions, namely, by the electric field strength and temperature. Oscillations in the GHz range are stable at low temperatures. The C_{60}^{+} oscillation frequency falls in the THz range after the temperature increase to 300 K. However, the oscillations are generated only at the external field of 10 V/μm and more. If the temperature is increased above 300 K, even larger electric field strength is necessary to generate stable oscillations in the THz range. Otherwise, if there is no technical possibility to increase the field strength, similar results can be obtained with the strength of 1 V/μm and by the placing a double charge on the fullerene molecule.

Adjusting the field strength allows controlling the oscillation frequency. The next step for the development of the THz nanoemitter will include location of the proposed peapod structure in the electric field and detection of the signal from the moving charged fullerene C_{60}. This task is practically implementable and can be realized using a thin C_{60} film hydrogen-annealing treatment [7].

IV. Acknowledgments

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