Modeling of current generation process in an aligned carbon nanotube under the action of strain gradient

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Abstract. The results of theoretical and experimental studies of the current generation process in an aligned carbon nanotube (CNT) during its deformation are presented. It is theoretically established that there is a strain gradient equal to 8 in the aligned nanotube under the influence of the external field strength of $10^{10}$ V/m. The piezoelectric coefficient of the CNT at a diameter of 92 nm and a length of 2.2 µm is empirically determined and amounted to 0.107 C/m$^2$. It is theoretically established that a CNT strain gradient of 8 leads to a current generation of up to 12 nA. It is shown that the modeling results correlate with experimental data. The obtained results can be used to develop the nanopiezotronics devices based on aligned carbon nanotubes.

1. Introduction
The new physical effects are observed in the materials on going from bulk to nanoscale [1]. Manifestation these physical effects led to the emergence of new areas for research. One of these areas is nanopiezotronics, which is aimed at creating electronic devices based on the use of the electromechanical effects in nanoscale materials [2-4]. One of the promising materials for creating nanopiezotronic devices is carbon nanostructures [5-10]. In the normal state, carbon cannot exhibit piezoelectric properties. However, the electric polarization is observed in carbon nanostructures with broken symmetry of the atomic lattice [6, 11, 12]. As a result, the carbon nanostructures exhibit the piezoelectric and flexoelectric effects [1, 6, 13, 14]. The breaking the symmetry of the carbon lattice can be carried out in various methods. One of the simplest and most promising methods is the formation of deformation in aligned carbon nanotubes (CNTs) by the application of a nonuniform electric field or local mechanical stress [6]. At the same time, it is shown that the electric current is generated in the aligned carbon nanotubes under the action of strain gradient [9, 10]. This fact can be used for the creation the fundamentally new devices of nanopiezotronics [8-10, 15, 16]. This research direction is actively developed now [15-19]. One of the main tasks of the current stage of research is the theoretical basis and modeling of the generation process of a piezoelectric current in carbon nanotubes under the action of mechanical stresses.

The aim is theoretical and experimental studies of the current generation process due to strain gradient in an aligned carbon nanotube.

2. Theoretical studies
The theoretical calculation of the current generated in the CNT under the action of strain gradient was based on the process of polarization of materials under the action of piezo-and flexoelectric effects:

$$j = \frac{\varepsilon_{ii}}{\varepsilon_{ii} - 1} \left( b \frac{\partial \Delta L(L, t)}{\partial t} \frac{1}{L} + b_f \frac{\partial^2 \Delta L(x, t)}{\partial x \partial t} \frac{1}{L} \right)$$  (1)
when \( j \) generates current, \( \varepsilon_{\parallel} \) – longitudinal dielectric constant of a CNT [11], \( b \) – piezoelectric coefficient of a CNT, \( b_{fl} \) – flexoelectric coefficient of a CNT, \( \Delta L \) – deformation of a CNT along axis \( x \), \( L \) – length of a CNT.

Simulation of the CNT deformation process under the action of an external electric field was carried out taking into account the previously obtained results [6]. The strain gradient of a CNT (a diameter of 90 nm, a length of 2 µm and a Young’s modulus of 1 TPa) arising from the application of a voltage pulse from 0 to 10 V and a tunnel gap of 1 nm is shown in Figure 1(a). The solution of the equation (1) is shown in Figure 1(b) for the strain gradient at \( \varepsilon_{\parallel} = 8 \) [20], \( b_{fl} = 10^{-10} \text{ C/m} \) [1, 18], \( b = 0.107 \text{ C/m}^2 \).

![Figure 1](image)

**Figure 1 (a, b).** (a) Theoretical time dependence of the CNT strain gradient on the external electric field. The insert presents the applied voltage pulse; (b) Theoretical time dependence of the current on the CNT strain gradient.

The piezoelectric coefficient \( b \) of a carbon nanotube with a diameter of 92 nm and a length of 2.2 µm was calculated empirically using the current-voltage characteristics of CNTs, which undergo deformation from 0.2 to 3 nm. Controlled elastic deformation in CNTs was formed under the action of a local electric field in the scanning tunneling spectroscopy mode [15]. The results of the study of elastically deformed CNTs showed that the largest hysteresis loop of the I – V characteristic is observed with CNT deformation of about 1 nm. This is due to the fact that the internal electric field which formed in CNTs having deformation of about 1 nm is completely redistributed due to the piezoelectric effect when external electric field is applied [9]. The hysteresis of the I – V characteristic decreases with a deviation from this deformation value [9]. This is due to the fact that the internal electric field of the CNT was insufficient for the formation of its high resistance state at deformation value of less than 1 nm. When CNT deformation is more than 1 nm, on the contrary, the resistance of CNTs in the low-resistance state increased due to a sharp increase in its internal electric field [9]. Hence, we can conclude that the internal electric field of CNTs with a diameter of 92 nm and a length of 2.2 µm tends to zero under conditions a deformation of 1 nm and a voltage of 8 V. Then the intrinsic resistance of the CNT is about 25 MΩ. Then, the resistance of CNTs in the low-resistance state increases to 202–285.7 MΩ with an increase in the deformation to 1.5–2.0 nm, respectively. If we assume that the increase in the resistance of CNTs is associated with an increase in the internal electric field of the CNT due to the manifestation of the piezoelectric effect, that the piezoelectric coefficient of the CNT with a diameter of 92 nm and a length of 2.2 µm is \( 0.107 \pm 0.032 \text{ C/m}^2 \).

Theoretical studies have shown that the strain gradient of CNTs increases from 0 to 8 when a sawtooth voltage pulse with an amplitude of 10 V is applied (Figure 1a). In this case, the value of the piezoelectric current of the generated CNT exponentially increases from 0 to 12 nA (Figure 1b).
3. Experimental studies

Array of aligned carbon nanotubes with a diameter of 92 nm, a length of 2.2 µm and a Young’s modulus of 1.4 TPa is grown by plasma-chemical vapor deposition using the multifunctional nanotechnological complex NANOFAB NTK-9 (NT-MDT, Russia). The scanning electron microscope (SEM) image of an experimental array of aligned CNTs is presented in Figure 2(a). Experimental studies of current generation in the CNT were carried out by atomic force microscopy (AFM) on the basis of the previously developed technique [6]. A force value applied to the AFM probe varied from 0 to 415 nN. The current dependence of the CNT deformation process is shown in Figure 2(b).

![Figure 2 (a, b). (a) SEM image of the CNT array; (b) Experimental time dependence of the current on the CNT strain gradient. The insert presents schematic of the measurement process.](image)

The results of experimental studies of the piezoelectric current of CNTs showed that the current does not flow in the "lower electrode/CNT/AFM probe" system, when the AFM probe is approached to the nanotube top (the approach section in Figure 2b). It is due to the CNTs do not undergo deformation in the initial state. When the pressure force is gradually applied to the AFM probe from 0 to 415 nN, there is a current with value from 0 to -18 nA, respectively (Figure 2b). With a decrease the pressure force back to 0 nN, the current value gradual decreases back to zero (Figure 2b). An insignificant current jump at t = 2 s is associated with a change in the type of CNT deformation from bending to tension under the action of adhesive forces holding the CNT top on the AFM probe during removal [6].

It was found that the current flows in the system "lower electrode/CNT/AFM probe" up to 18 nA. The obtained values correlated well with the theoretical studies.

4. Conclusion

Thus, the theoretical and experimental studies of the current generation process due to strain gradient in an aligned carbon nanotube were carried out. It is theoretically established that a strain gradient equal to 8 is formed when an external electric field about $10^{10}$ V/m is applied to the CNT with a diameter of 90 nm, a length of 2 µm and a Young’s modulus of 1 TPa. Experimental studies of the I-V characteristics of CNTs with different strains are carried out. Analysis of these dependencies allowed us to evaluate the piezoelectric coefficient of the CNT with a diameter of 92 nm and a length of 2.2 µm which amounted to $0.107 \pm 0.032 \text{ C/m}^2$. The simulation results showed that the current value can reach up to 12 nA for the CNT with strain gradient at 8 and piezoelectric coefficient to $0.107 \pm 0.032 \text{ C/m}^2$. The theoretical results are confirmed by experimental studies. It is confirmed the adequacy of the modeling. The obtained results can be used to develop the nanopiezotronics devices based on aligned carbon nanotubes.
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