Theoretical study of the photoconductivity mechanism of the structure “carbon nanotubes – silicon substrate”

V.S. Pavelyev[1], A.V. Mezhenin[1], M.A. Sovetkina[1], A.R. Rymzhina[1]

[1]Samara National Research University, Moskovskoye Shosse 34A, Samara, Russia, 443086

Abstract. The types of optical radiation photodetectors have been considered according to the operating principle. The photoconductivity mechanism of carbon nanotubes (CNTs) deposited on a silicon substrate has been investigated theoretically. A comparison of the CNTs band gap with illuminating beam the quantum energy has been conducted. The heating and cooling cycles under the influence of a distributed surface energy source have been simulated. It has been established that CNTs on a silicon substrate have thermal-type photoconductivity. The sensitive element of the IR sensor based on this structure can be classified as a bolometric type.

1. Introduction

Currently, there is a fairly broad classification of optical radiation receivers. According to Ref. [1], they are divided into three large groups depending on the physical phenomena underlying the operating principle: photovoltaic (photon-assisted), photoelectronic, and thermal. Photovoltaic radiation receivers are based on the internal photoelectric effect. In photoelectronic devices, the physical operation principle is the external photoelectric effect. The heat radiation receivers operation is based on the change in a resistance of a sensitive element with the increasing in its temperature under the action of the absorbed radiation.

Heat radiation detectors are non-selective devices, i.e. they have the same spectral characteristic in a wide range of the electromagnetic spectrum. The work of such receivers is based on the conversion of radiation energy first into thermal and then into electrical ones. Photovoltaic and photoelectronic receivers are selective devices, i.e. they have a sensitivity only in a certain range of the electromagnetic spectrum. Receivers with the internal photoelectric effect use three main physical phenomena caused by the action of radiation on a semiconductor: the photoconductivity phenomenon, photovoltaic and photoelectric effects [2].

Photovoltaic radiation detectors are based on the internal photoelectric effect and the semiconductor manufacturing technology. Photoresistor, photodiode, phototransistor, and photothyristor structures made of a semiconductor material sensitive to radiation in the operating spectral region are used as a photosensitive element in photodetectors. In photoelectronic devices, the electron flow (beam) moves under the action of an electric field in a vacuum or gas-filled apparatuses.

Thermal optical radiation receivers are divided into pyroelectric (pyroelectric detectors) and semiconductor (bolometers). Pyroelectric radiation detectors are based on the pyroelectric effect which arises as a result of change in the pyroactive crystal temperature due to the absorption of radiation energy. If a change in the electrical resistance of a conductor or semiconductor is caused by a change in temperature, then the receiver is called bolometric (the bolometer) [1].

Commercially available detectors require special operation conditions, for example, a cryogenic temperature or a sealed housing that is often due to the sensor material properties [1]. Their sensitivity increases continuously and the photodetectors sensitivity spectrum expands beyond the visible region to the optical range limits at the same time [3]–[6]. The requirements for the detector sensitive element include: low inherent noise level, small pixel size [6], low cost, large area (more than 5×5 mm^2) and quick response [7]. For the bolometric type IR-sensor, it is very important to reduce the thermal noise because it complicates the work of a detector at temperatures above the room temperature [3], [4].

Increasing the degree of integration, rising in the response rate, and toughening operating conditions precondition a constant search for new, cheap, and technological materials. One of the promising materials for the detector sensitive element is carbon nanotubes (CNT). Currently, they are considered as a potential candidate for the replacement of existing materials in virtually every field. The properties of CNTs can be controlled by changing their structure. Thus, the transition metals embedding leads to a sharp increase in the conductivity of both semiconductor CNTs (due to the electronic states appearance of the metal within the band gap) and metallic CNTs (due to the increase in the states density near the Fermi level) [7].

In nanotechnology, CNTs can be sensors for registering various physical and chemical effects; probes for scanning microscopy and atomic manipulators; nanowires, nanoresistors, nanotransistors, nano-optical elements for the new generation nano-optoelectronics, etc. The main reasons for their wide distribution are associated with their unusual size and size-dependent physical properties [8], [9]. In terms of IR-sensors, the unique feature of CNTs is the ability to control the operating parameters through the changing of their structure: expansion of the absorption spectrum, selective tuning to the required wavelength, etc.

The principal opportunity of using a two-layer CNTs–silicon substrate structure as a sensitive element for detection the monochromatic radiation of visible light-emitting diodes was shown in Ref. [7]. In work [10], similar samples were used as the detector for the sensing of far IR-range radiation. It was observed a decrease in the samples resistance with the increasing of illuminating beam power. The dynamic range and transient characteristics of the sensor to be created were determined. However, it is necessary to carry out the theoretical investigation of photoconductivity mechanisms of the CNTs–silicon substrate structure for a successful production of such sensors. It is the purpose of the present work.

2. Sensitive element working conditions simulation

A decrease in the resistance of the structure under study at the far-IR range monochromatic radiation influence can be occasioned by two factors – an increase in the charge carriers concentration in the CNT-layer volume or an increase of their mobility. In this regard, we consider both possible mechanisms of the conductivity change.

The generation of charge carriers within the framework of the first mechanism is possible if the quantum energy of the illuminating beam exceeds the band-gap of the nanotubes. According to Ref. [11], the band gap E_g decreases with an increase in the CNT diameter d_{CNT} (external in the case of multi-walled CNT) in accordance with the dependence given in figure 1. It was found in Ref. [10] that the characteristic size of multi-walled nanotubes is in the range of 10–20 nm. Consequently, the band gap is 0,07 eV or 10^{-20} J.

The condition of the charge carriers growth due to the internal photoelectric effect can be written as

$$h\nu \geq E_g, \tag{1}$$

where $h\nu$ is the quantum energy of infrared radiation. Considering that the frequency ν is related to the wavelength by the formula

$$\nu = c/\lambda, \tag{2}$$

where c is the speed of light in vacuum, we find $h\nu=1.9\cdot10^{-20}$ J.

Based on this, in Ref. [10] it was concluded that the generation of charge carriers in CNTs is theoretically possible due to the internal photoelectric effect. However, the quantum energy of the illuminating beam exceeds the band-gap slightly, and the states density at the bottom of the conduction band may not be enough to significantly reduce the sample resistance. Therefore, it is reasonable to check another mechanism.

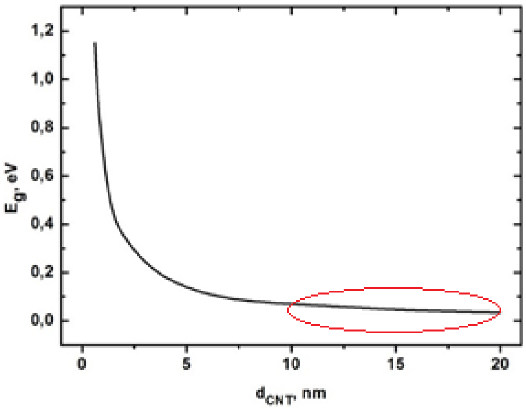


Figure 1. The dependence of the band-gap on the CNT diameter (the range determining the characteristic size of nanotubes in Ref. [10] is marked in red).

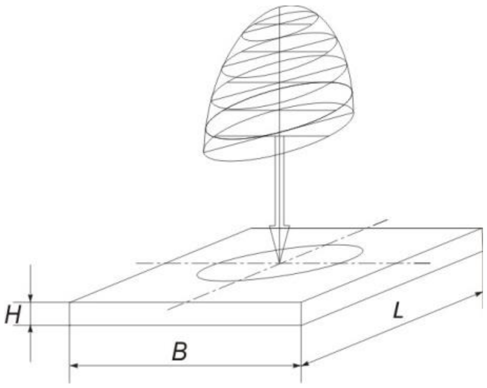
Let us determine the contribution to the charge carriers generation associated with an increase in the substrate temperature. When laser radiation illuminates the CNT–silicon substrate structure, a part of the energy is absorbed by the crystal lattices of the layers. As a result, the temperature of this structure changes. The establishment of a temperature fields dynamics in the sensitive element volume during heating and cooling allows us to relate the receiver on the basis of the considered structure to the photon-assisted or bolometric type.

Modern physical modeling facilities (ANSYS, COMSOL, etc.) make it possible to calculate heating and cooling processes quickly and efficiently. A thermal fields formation is determined by the parameters of the energy source, material properties, exposure time, and heat exchange conditions with an environment.

It has been assumed that the CNT network has a small thickness, which permits to consider it as a coating on a silicon substrate. We suppose also that the nanotubes completely absorb the radiation impinging on them, that is they have optical properties characteristic of an absolutely black body. The nanotubes remain in direct thermal contact with the substrate, which is a massive body compared to them. We think that a rapid heat exchange between the nanotubes and the substrate caused by the thermal conductivity takes place when radiation is falling. This circumstance leads to an instant achievement of their temperatures levelling-off.

A heating-cooling cycles simulation for the sample of CNTs deposited on a silicon substrate was carried out according to the scheme presented in figure 2 under the conditions similar to experimental those described in Ref. [10]. Since the sample is a silicon substrate with nanotubes network located on its surface several tens of microns thick, it is accepted that the object under study is characterized by the substrate dimensions $L \times B \times H$=10×10×0.5 mm. The affecting energy source is placed in the center of the upper bound. The CNTs network, in essence, is a coating on silicon piece that monitors the change in the energy of a massive body, which is a substrate. Therefore, we use the parameters of silicon as the thermophysical characteristics of the material in this task.

To calculate the temperature fields, it is reasonable to use the ANSYS software package [12]. It is a universal system of finite element analysis intended, in particular, for solving problems of heat transfer and heat exchange. The finite element method is implemented for the numerical solution of problems in the ANSYS. The decision itself is carried out within a specific project. The project is formed by adding in its structure the corresponding moduli, filling them and a connection with subsequent moduli those produce further processing, until the result will have obtained. The task description is carried out in accordance with the selected project schematics in the following sequence: setting the material and its properties, an object geometry attachment, a mesh generation, an assignment of initial and boundary conditions and energy source parameters.



L – length, B – width, H – height

Figure 2. Model experiment schematic.

In this case, the modeling process is divided into two subtasks – heating simulation and cooling simulation. In the first, a beam with the diameter of 5 mm illuminates the sample. The energy source is characterized by a circular Gaussian power density distribution within the aperture. To reproduce the full-scale experiment conditions, the results of a temperature field calculation at the heating stage are taken as the initial for cooling process modeling. In the second subtask, the exposing energy source is absent. Cooling determined by the natural convection. The thermal load value stepwise changes at the end of a heating-cooling cycle, and a new cycle is counted with new energy source parameters.

Figure 3 shows the result of the heating stage simulation at the exposure radiation power of 1 W. Analysis of the temperature field allows us to conclude that the entire substrate is heated uniformly, since the difference between the maximum substrate temperature at the center and the minimum at the periphery is only 0.003°C.

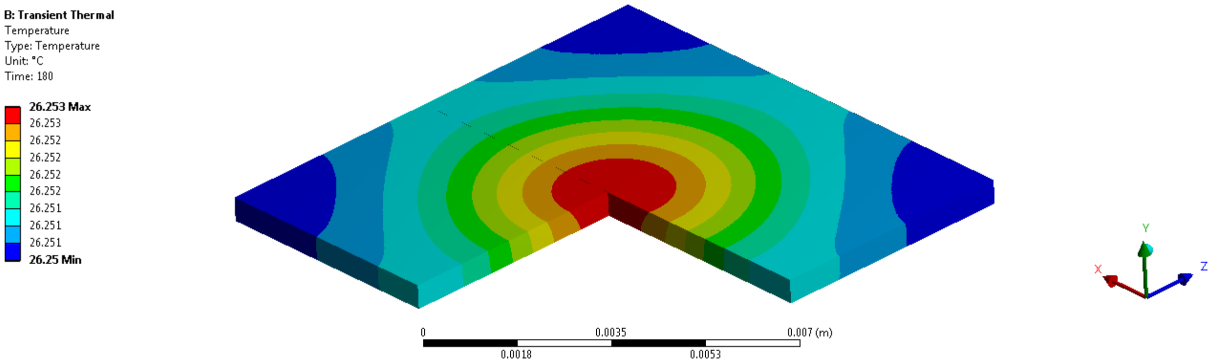


Figure 3. The temperature field within the sample at the end of the heating stage (t=180 s) at the exposure radiation power of 1 W.

Cooling stage simulation allows us to state the complete uniformity of the temperature field after 3 min since the end of radiation exposure. Figure 4 shows the calculation results of the temperature field, as an example.

Figure 5 presents the calculation results for the maximum temperature change inside the sample volume for six heating-cooling cycles corresponding to the thermal loads values at the heating stage. We can see the nonlinear temperature behavior, a rise at the heating and a decrease at the cooling stages. The maximum sample heating during the heating-cooling cycles does not exceed 4°C even if the irradiating source power is W=3 W.

The increase in the electron energy due to the transfer to it the vibrational energy of the atoms composing the crystal lattice is about 0.5% of the band-gap. This is clearly not enough to change the charge carriers concentration in the conduction band. However, this is significant for the mobility increasing of the electrons already existing in this zone.

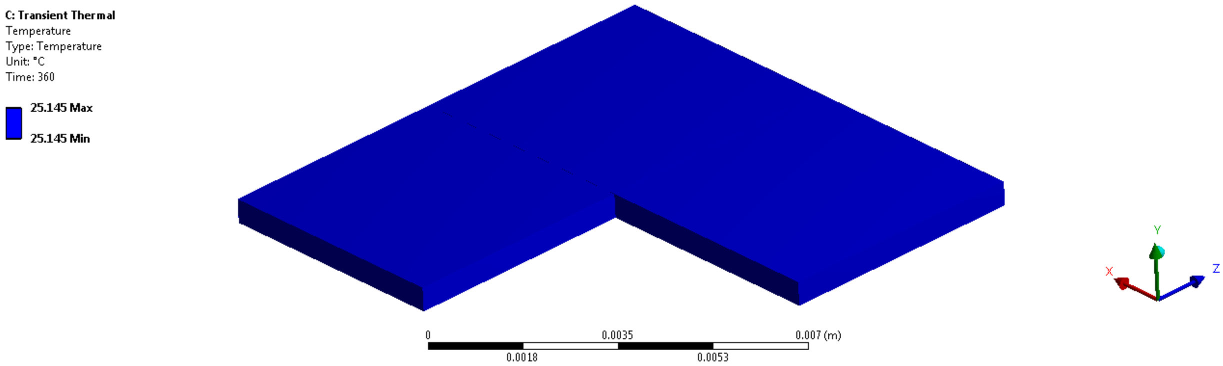


Figure 4. The temperature field within the sample at the end of the cooling stage (*t*=360 s) at the exposure radiation power of 1 W during the heating stage.

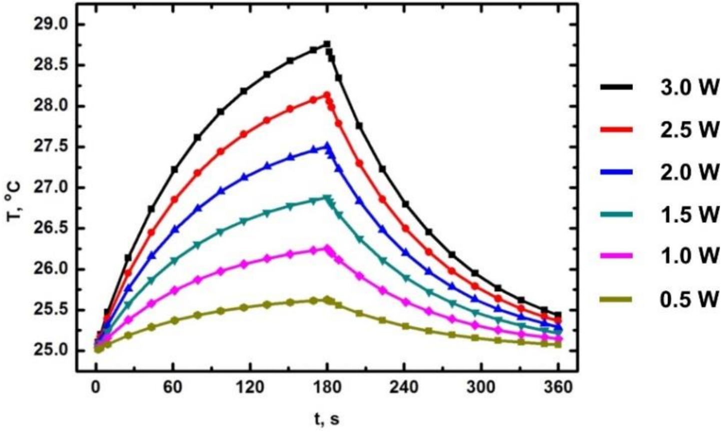


Figure 5. Dependence of the maximal sample temperature on time.

Comparison of the character of the temperature curves shown in figure 5 with the resistance behavior of the samples (figures 10 and 11 in Ref. [10]) at various power levels permits to conclude that the rise and decrease in the conductivity of the sample over time caused namely by a nonlinear change in its temperature.

3. Conclusion

A classification of optical radiation photodetectors according to the operation principle is given, and the requirements for the sensitive elements of optical radiation detectors are revealed. It is shown that CNTs are a promising material for IR-sensors.

Possible mechanisms of changing the conductivity of the sensor based on the "CNT–silicon substrate" structure are considered. It is established that the increase in the sensor conductivity caused by the charge carriers generation due to the interband transition is insignificant. Consequently, the photoconductivity changing mechanism of the structure under study does not fundamentally allow us the classification of a sensitive element as photon-assisted.

Numerical simulation of the temperature field dynamics shows that the increase and decrease in resistance occur due to temperature changes, which makes it possible to classify the IR-sensor based on the "CNT–silicon substrate" structure to the detector of bolometric type.

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