

A Mathematical Model for a Radon Detection Method Based on Carbon Nanotube Sensor

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Abstract—This article is proposing a mathematical model as a basis for radon detection by measurement alpha particle concentration with a carbon nanotubes-based sensor. The working principle at the basis of the mathematical model of the presented sensor is based on the fact that, the concentration of alpha particle in the air is a linear function of radon concentration. The collision between each alpha particle and the attachment of alpha particle to the carbon nanotube, changes the nanotube's own oscillation frequency. After activation, the carbon nanotubes oscillations in frequency depends on their own geometrical dimensions and their mechano-electrical properties. The initial oscillation frequencies spectra of the matrix of carbon nanotube with the same geometrical dimension is compared with the oscillation frequency spectra collected after the sensor is exposed to air sample. Based on their relative frequency variations of the recorded spectra, the radon concentration is evaluated. Radon concentration is determined on the bases of the linear relationship between its concentration and the alpha particles one. According to these theoretical assumptions, the use of carbon nanotubes sensor appears to be suitable for radon concentration measurement with the advantages to be a reusable and a low cost solution.

Keywords—carbon nanotubes, sensor, radon, alpha particle.

I. INTRODUCTION

European Directive 59/2013 EUROATOM establishes the basic safety rules on protection against the dangers arising from the exposure to ionizing radiation [1]. The international concerns came in the context in which Radon can lead to bronchopulmonary cancer. International Agency for Research on Cancer (IARC/OMS) has classified Radon gas as a carcinogenic agent of group 1 (verified carcinogenic for human) [2]-[4]. Radon gas accumulation is determined mainly by uranium/radium concentration into the soil as well as in building materials [5],[6]. Radon (Rn) is a radioactive gas, from group 18 of the periodic table (noble gas), generated by the radioactive decay of radium. Radon is a colorless gas, 7.5 times heavier than air and 100 times heavier than hydrogen. It liquefies at -61.8°C (-79.2°F) and freezes at -71°C (-96°F).

Radon is rare in nature because its isotopes have short lifetimes and radium is a scarce element. The atmosphere contains traces of radon near to the ground due to the decomposition of radium present in the soil and rocks.

Radon occurs naturally as a decay product of uranium present in various types of rocks.

Due to its presence in the soil, building and insulation materials, radon becomes dangerous in closed, unventilated spaces such as basements of buildings, historical monuments, churches and even work and living spaces. One of the objectives of Vienna International Agency is the Radon map for entire Europe (currently still not completed in Romania).

There are active and passive methods for the monitoring of the radon level implemented in several devices often expensive or that needs for a post processing in specialized laboratories of the sensing element. Measurement instruments based on active method include electret ion chambers, scintillation chamber and superficial barrier devices, the ones based on passive method include alpha track detectors, active carbon absorption detector and electronic detector [5].

Radon has a half-life of 3.8 days. When radon is inhaled, the short-lived descendants of radon (^{218}Po and ^{214}Po), which have a very short half-life (3.1 minutes and 0.16 milliseconds, respectively), reach the lungs and emit alpha particles that interact with the tissue and can causes transformations or damage to cells [7]-[13].

In this article, we propose a mathematical model of carbon nanotube sensor for the measurement of Radon gas (^{222}Rn). The carbon nanotubes change their oscillation frequencies under the interaction with the heavy nuclei of alpha particles, positively charged, attracted by the nanotube negatively charged. This allows to design a sensor for monitoring the level of Radon pollution present in the surrounding area [14]. The use of carbon nanotube sensor for monitoring the level of radon gas indoor will be a low cost solution and an appropriate mean of applied circular economy working principle. Indeed, the nanotube sensor is reusable after thermal discharge [15]. As a consequence, it is suitable to equip smart object and then for the developing of distribute monitoring systems based on Internet of Things [16]-[21].

Unless, there is not yet a complete radon map of Europe, as a consequence it is not possible to estimate the risk for public health in most of the areas of living residences as well as for public and working places. The low cost sensor will allow to overcome this lack of information. Moreover, thanks to IoT paradigm the smart object based on nanotube sensors can be developed and easily added in IoT systems already available for the monitoring of the structures [22]-[24] or to equip UAV systems [25].

II. A MODEL OF A SENSOR WITH CARBON NANOTUBES FOR ALPHA PARTICLES CONCENTRATION.

The analysis model proposed in this paper deals with the detection of alpha particles resulted from the decay of ^{222}Rn by using a carbon nanotube sensor. In this sensor, the attached end of the carbon nanotubes is connected to a cathode substrate, which make possible the accumulation at the free end of the alpha particles. This will allow an indirect measurement of the amount of radon gas in the vicinity of the detector.

Indeed, the oscillation frequencies of the nanotubes are measured, and the spectrum of the nanotube frequencies is compared before and after the attachment of the alpha particles. By measuring the relative variation of the frequency following the coupling of the alpha particles, the detection can be made at the level of a single alpha particle. Due to the high elasticity ($E=10^{12}$ Pa) of the nanotubes a tiny change in mass produces a high frequency variation of the nanotube.

III. THE MATHEMATICAL PATTERN FOR THE CARBON NANOTUBE USED AS A SENSOR FOR ALPHA PARTICLES

The carbon nanotube behaves as an elastic homogeneous bar submitted to oscillations because it is fixed at one end meanwhile the other one is free. Submitted to piezoelectric activation the carbon nanotube will oscillate freely in the y direction. We consider nanotube oscillation by the approximation of small oscillations that can be express by [26]-[29]:

$$EI \frac{\partial^2 u_y}{\partial x^2} + \rho A \frac{\partial^2 u_y}{\partial t^2} = 0 \quad (1)$$

where E is the Young module of elasticity of the carbon nanotube, I is the moment of inertia of the nanotube, ρ is the average density of the carbon nanotube, A is the cross-sectional area of the carbon nanotube at a distance x from O , and u_y is the elongation of the nanotube at the coordinate point x .

Equation (1) shows that any point of the bar oscillates harmonically in the uncamped case, which allows us an analogy between the oscillation of the free end of the bar and the oscillation of an elastic pendulum.

The bar subjected to unamortized free oscillations can be modeled as a discrete system- the elastic pendulum – in which the bar is considered without mass and the whole mass is concentrated at its free end. The equation of motion for this elastic pendulum model is:

$$-k_{ech}y = m_{ech} \frac{d^2 y}{dt^2} = -4\pi^2 \nu^2 m_{ech} y \quad (2)$$

where k_{ech} is the elastic constant of the pendulum and m_{ech} is its equivalent mass.

The natural frequency of the oscillator equivalent to the carbon nanotube, in the case of small oscillations can be expressed by the relation:

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k_{ech}}{m_{ech}}} \quad (3)$$

The analogy criteria derive from the condition that the elastic pendulum has the same oscillation frequency as the free end ($x = L$) of the nanotube, so:

- the elastic constant of the pendulum must be the factor of proportionality between the maximum force exerted on the free end of the bar and its amplitude of oscillation;
- the mass of the pendulum must correspond to the equality between the maximum kinetic energy of the bar and the maximum kinetic energy of the pendulum.

The problems to solve are:

1. What is the elasticity constant k_{ech} of the equivalent spring?
2. What is the mass m_{ech} of a body caught by the equivalent spring that oscillates with the same frequency as the nanotube?

An additional mass attached to the end of the carbon nanotube will change the frequency of its small oscillations.

To solve the first problem, we will use the resistance equations of the materials from Timoshenko and Gere [29], Timoshenko and Young [30], and to solve the second problem we will use an approach equivalent to that used by Zacarias, Wang and Reimbold in [31].

A. The carbon nanotube shaped like a linear elastic body

Static bending deformation of nanobars

Let be a nanotube with a recessed end, subjected to bending. We define the infinitesimal element in the nanotube delimited by two cross sections in the nanotube through the x and $x + dx$ coordinate points, respectively (as in Fig. 1)

Note, $F_s(x)$, respectively, $F_s(x + dx)$ the shear forces in the two cross sections, j is the versor of the Oy and k is the versor of the Oz axis.

$F_s(x) = -F_s(x)j$, $F_s(x + dx) = F_s(x + dx)j = [F_s(x) + dF_s]j$ and $f_l(x)$ is the force on the unit length along the nanobar distributed on the length dx , $f_l(x) = f_l(x) \cdot j$, axis.

The bending moments $M(x)$, respectively, $M(x + dx)$ are directed along the Oz axis $M(x) = M_z(x)k \equiv M(x)k$, $M(x + dx) = -M(x + dx)k \equiv -M(x + dx)k = [M(x) + dM(x)]k$.

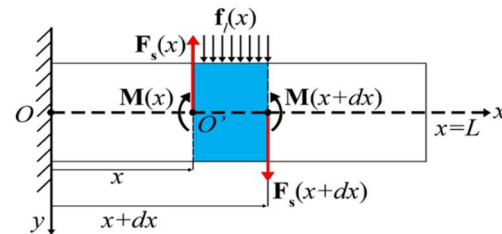


Fig. 1. Infinitesimal element in the embedded nanotube, subjected to bending

Problem 2.1: Let consider a nanotube with a recessed end be subjected to bending. Determine the elastic constant of the nanotube (the proportionality factor between the maximum force exerted on the free end of the nanotube and its amplitude of oscillation).

The global equilibrium and written conditions for the infinitesimal element represented in Figure 1 are:

$$f_l(x)dx + (F_s + dF_s) - F_s = 0$$

$$\text{or} \quad \frac{dF_s}{dx} = -f_l(x) \quad (4)$$

and

$$\begin{aligned} & [M(x) + dM(x)] - M(x) - \\ & - [F_s(x) + dF_s]dx - \frac{1}{2} [f_l(x)dx]dx = 0 \end{aligned}$$

or

$$\frac{dM(x)}{dx} = F_s(x) \quad (5)$$

where $M(x)$ is the moment in position x along the nanobar.

Let us now evaluate the deformation of a section of the nanobeam in the bend (Fig. 2.).

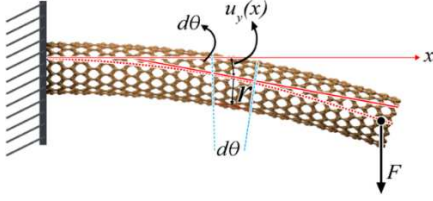


Fig. 2. Nanotube modeled as a nanobeam.

In a section located at x , the nanobar has a radius of curvature $R(x)$, and the neutral axis of the infinitesimal element dx has the length $dx = R(x) d\theta$ and underlies the angle $d\theta$. At the distance r from the neutral axis, the infinitesimal element has the length:

$$dl = [R(x) - r] d\theta \equiv R(x) \left[1 - \frac{r}{R(x)} \right] d\theta \quad (6)$$

Thus, the length of the infinitesimal elementary segment under tension is:

$$dl = dx - \frac{r}{R(x)} dx \quad (7)$$

Therefore, the deformation ($\epsilon = \epsilon_{xx}$) can be expressed as:

$$\epsilon_{xx} = \frac{dl - dx}{dx} = -\frac{r}{R(x)} \quad (8)$$

and the stress-strain relationship in the theory of linear elasticity, $\sigma_{xx} = \epsilon_{xx} E$, leads to:

$$\sigma_{xx} = -\frac{r}{R(x)} E \quad (9)$$

Denoting by A the area of the cross section in the nanotube and considering an infinitesimal element of it, located at a distance r from the neutral axis, of length $l(r)$ (as in Fig.3)

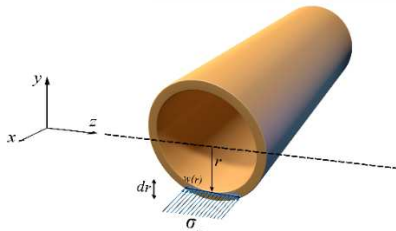


Fig. 3. Nanobar cross section

Calculate the resulting internal bending moment with respect to O' , using (9):

$$\begin{aligned} M_z &= \int \sigma_{xx} \ell(r) r dr = \int \frac{-E}{R(x)} \ell(r) r^2 dr = \\ &= -\frac{E}{R(x)} \int \ell(r) r^2 dr = -\frac{E}{R(x)} I \end{aligned} \quad (10)$$

where

$$I = \int \ell(r) r^2 dr \quad (11)$$

I is the moment of inertia.

From (10) it follows that the resulting internal bending moment thus depends on the local radius of curvature of the bar, $R(x)$.

Noting by the displacement of the nanotube considered as a function of x , we can express the local radius of curvature of the bar, $R(x)$, by the relation:

$$\frac{1}{R(x)} = \frac{\frac{d^2 u_y(x)}{dx^2}}{\left[1 + \left(\frac{du_y(x)}{dx} \right)^2 \right]^{3/2}} \quad (12)$$

For the bending of nanotubes, used as nanosensors, we will consider that, $\frac{du_y(x)}{dx} \ll 1$, and so we will approximate:

$$\frac{1}{R(x)} = \frac{d^2 u_y(x)}{dx^2} \quad (13)$$

Using equation (10), we obtain:

$$\frac{d^2 u_y(x)}{dx^2} = -\frac{M(x)}{EI} \quad (14)$$

Differentiating equation (10) and using equation (13)

$$\frac{d^3 u_y(x)}{dx^3} = -\frac{F_s(x)}{EI} \quad (15)$$

Differentiating once again and using equation (4), we obtain the bending bar equation which expresses the dependence of the bar deformation $u_y(x)$ on the force distribution, $f_l(x)$,

Observation:

The equation given by Timoshenko and Young [30] which defines the bending of the nanotube under the action of forces directed in the direction of Oy , is represented by:

$$EI \frac{d^4 u_y(x)}{dx^4} = f_l(x) \quad (16)$$

The conditions associated with the Cauchy problem, in the so-called "embedding" conditions of the bar are:

$$u_y(0) = 0 \quad (17)$$

$$\frac{du_y(0)}{dx} = 0 \quad (18)$$

$$\frac{d^2u_y(L)}{dx^2} = 0 \quad (19)$$

This equation is useful when determining the geometrical configuration of the bar when only external loads are involved.

B. The moment of inertia for a carbon nanotube

Consider a cross section in a carbon nanotube (as in Fig. 4). The moment of inertia of the nanotube expresses by:

$$I = \int_{R_i}^{R_e} \int_0^{2\pi} r^2 \sin^2 \theta (r d\theta dr) = \int_{R_i}^{R_e} \int_0^{2\pi} r^3 \left[\frac{1}{2} - \frac{1}{2} \cos(2\theta) \right] d\theta dr = \pi \frac{R_e^2 - R_i^2}{4} \quad (17)$$

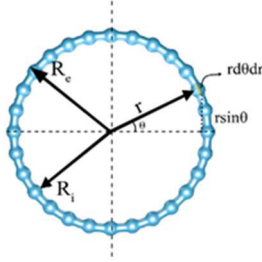


Fig.4 A cross section of the carbon nanotube.

C. The charging point at the free end of the nanotube

The solution of the Cauchy problem (16) with the associated conditions (17) - (19) in the case of a point load applied to the nanotube:

$$f_l(x) = -F\delta(x-L) \quad (20)$$

Replace the Dirac distribution in Equation (20) with a function support with compact support and zero to the size of the compact support in the determined solution. Integrating the equation (16), we obtain:

$$\frac{d^3u_y(x)}{dx^3} = -\frac{F}{EI} + C \quad (21)$$

Comparing this result with equation (15), we obtain:

$$C = \frac{2F}{EI} \quad (22).$$

We integrate (21) and taking into account (22), we obtain:

$$\frac{d^2u_y(x)}{dx^2} = \frac{F}{EI} x + C' \quad (23)$$

Given the condition (19), it follows that:

$$C' = -\frac{FL}{EI} \quad (24)$$

We integrate (23) and taking into account (24), we obtain:

$$\frac{du_y(x)}{dx} = \frac{F}{2EI} x^2 - \frac{FL}{EI} x + C'' \quad (25)$$

Introducing in the condition of (18) into (25) we obtain:

$$\frac{du_y(x)}{dx} = \frac{F}{2EI} x^2 - \frac{FL}{EI} x \quad (26)$$

After integrating the equation (26), we obtain:

$$u_y(x) = \frac{F}{6EI} x^3 - \frac{FL}{2EI} x^2 + C''' \quad (27)$$

Putting in the equation (27) the condition (17) we obtain $C''' = 0$, and from (27) we deduce:

$$u_y(x) = \frac{F}{EI} \left(\frac{x^3}{6} - \frac{Lx^2}{2} \right) \quad (28)$$

The elastic constant of the spring equivalent to the trapped nanotube is determined by evaluating the maximum deformation that occurs at the free end of the nanotube:

$$F = -\frac{EI}{3L^3} u_y(L) = -k_{ech} u_y(L) \quad (29)$$

so the equivalent elastic constant is

$$k_{ech} = \frac{EI}{3L^3} \quad (30)$$

D. Determination of the mass of the oscillator equivalent with the carbon nanotube

Problem 2.2: Let a nanotube with an embedded end oscillate after (1). Determine the mech mass of an oscillator caught by the described equivalent spring by which it oscillates at the same frequency as the nanotube. Static deformation of the nanotube described in Problem 2.1. it is assimilated to the dynamic problem:

$$m_{ech} \frac{d^2 \mathbf{x}}{dt^2} = -k_{ech} \mathbf{x} \quad (31)$$

To solve this problem we will use an energetic method as in Zacarias et al. [31]. The method used to determine the equivalent mass, m_{ech} , is to make an energy analogy between the nanotube and the equivalent oscillator. The principle of equivalence is that the nanotube and the equivalent oscillator have the same dynamic effect, ie the same maximum kinetic energy.

Considering that the system consisting of the nanotube modeled as a nanobar and an attached mass m of an alpha particle is set in motion by oscillation. The maximum total kinetic energy of the system can be expressed as the sum of the maximum kinetic

energy of the carbon nanotube and the maximum kinetic energy of the α particle mass attached to its free end:

$$E_c^{total} = E_{CNT} + E_{alpha\ particle} \quad (32)$$

For the equivalent oscillator, the maximum kinetic energy can be expressed by the relation:

$$E_c^{total} = \frac{1}{2} m_{eq} v_{max}^2 \quad (33)$$

Applying the theorem of variation of the kinetic energy between the state of maximum deformation (in which the speed of the equivalent oscillator is zero) and the state of stable equilibrium of the oscillator (in which its speed is maximum), we obtain:

$$E_c^{total} = \frac{1}{2} m_{eq} \omega^2 \cdot y^2(L) \quad (34)$$

E. Determination of the maximum kinetic energy of the carbon nanotube

Noting with ρ is the density of the nanotube, A is the cross-sectional area and L its length, we can express the mass of an infinitesimal element of thickness dx in the carbon nanotube.

$$dm_{CNT} = \rho A dx \quad (35)$$

Applying the theorem of variation of the kinetic energy between the maximum deformation state (in which the infinitesimal element is zero) and the undeformed state of the nanotube (in which the speed of the infinitesimal element is maximum), the maximum kinetic energy of the infinitesimal element is:

$$dE_{CNT} = \frac{1}{2} \omega^2 u_y^2 dm_{CNT} = \frac{1}{2} \rho A \omega^2 u_y^2 dx \quad (36)$$

And the kinetic energy of the nanotube, according to (36) is:

$$E_{CNT} = \frac{1}{2} \int_0^L \rho A \omega^2 u_y^2 dx \quad (37)$$

Given the equation (27), it follows that (37) can also be expressed as:

$$E_{CNT} = \frac{1}{2} \int_0^L \rho A \omega^2 \left[\frac{Fx^2(3L-x)^2}{6EI} \right] dx = \frac{1}{2} \rho A \omega^2 \left(\frac{33L}{140} \right) \left(\frac{FL^3}{3EI} \right)^2 = \frac{1}{2} m_0 \omega^2 \left(\frac{FL^3}{3EI} \right)^2 \quad (38)$$

$$\text{Where: } m_0 = \frac{33L}{140} \rho A$$

F. Expression of the maximum kinetic energy of the mass m of alpha particle

By applying the theorem of variation of the kinetic energy between the maximum deformation state (in which the

infinitesimal element is zero) and the undeformed state of the nanotube (in which the velocity of the infinitesimal element is maximum), we obtain the maximum kinetic energy of oscillation mass of an alpha particle attached to the nanotube:

$$E_{alpha\ particle} = \frac{1}{2} m \omega^2 u_y^2(L) = \frac{1}{2} m \omega^2 \left(\frac{FL^3}{3EI} \right)^2 \quad (39)$$

Substituting (38) and (39) in (32) it is obtained:

$$E_c^{total} = \frac{1}{2} \omega^2 (m_0 + m) \left(\frac{FL^3}{3EI} \right)^2 = \frac{1}{2} \omega^2 (m_0 + m) \cdot y^2(L) \quad (40)$$

Comparing (34) with (40), it follows that an oscillating nanotube can be modeled as a spring of the k_{ech} elasticity constant and a m_{ech} equivalent mass body at its end given by the expression:

$$m_{ech} = m_0 + m \quad (41)$$

G. Expression of the oscillation frequency of the nanotube

Using the simplified body-spring model and the equations (1), (30) and (41) we can express the frequency of the carbon nanotube with a mass m of an alpha particle at its end by:

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k_{ech}}{m_{ech}}} = \frac{1}{2\pi} \sqrt{\frac{3EI}{(m_0 + m)L^3}} \quad (42)$$

If no alpha particle is attached, then the oscillation frequency of the nanotube is:

$$\nu_0 = \frac{1}{2\pi} \sqrt{\frac{3EI}{m_0 L^3}} \quad (43)$$

It follows from (42) and (43) that:

$$\nu = \nu_0 \sqrt{\frac{m_0}{m_0 + m}} < \nu_0 \quad (44)$$

The relative variation of the nanotube frequency following the attachment of the mass m of a particle is:

$$m = m_0 \left[\frac{1}{\left(1 + \frac{\Delta \nu}{\nu_0} \right)^2} - 1 \right] \quad (45)$$

The equation (45) allows the determination of the particle, or molecular species attached to the nanotube. Measuring experimentally the frequency ν_0 of the nanotube oscillation without particle attached, exposing the nanotube in the detection area where the evaluation sample is present, it can be measured the new value of the oscillation frequency ν .

Based on the same principle a detection sensor for any molecule, macromolecule (e.g. acetone from exhaled air in diabetic persons) [15], [26], [30], [32]-[34], present in the exhaled air can be identified and measured.

Under the hypothesis of non correlation among measurements of m_0 , Δv , and v_0 , the uncertainty of m is calculated by using:

$$u_m = \sqrt{\left(\left(\frac{1}{\left(1+\frac{\Delta v}{v_0}\right)^2} - 1\right) u_{m_0}^2 + \left(-\frac{2m_0}{v_0\left(1+\frac{\Delta v}{v_0}\right)^3}\right) u_{\Delta v}^2 + \left(\frac{2m_0\Delta v}{v_0^2\left(1+\frac{\Delta v}{v_0}\right)^3}\right) u_{v_0}^2\right)} \quad (46)$$

where u_{m_0} , $u_{\Delta v}$, are the uncertainty of m_0 , Δv , and v_0 , respectively.

IV. CONCLUSIONS

The new mathematical model here proposed will allow the design of Radon sensors based on nanotubes. The low cost of the sensor together with the possibility of reuse it several times seems to be a promising solution for a punctual mapping and monitoring of environment from Radon pollution. The importance of a punctual monitoring of Radon comes from the fact that it is the second cause of lung cancer after cigarette smoking. The measurement devices based on nanotube sensor would be cheap and reusable, and will be smart and easily integrable in the existing IoT systems. This will permit not only a more widespread monitoring, but also to easily make available this data to scientists, technicians, clinicians and laymen users through internet.

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