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# Rubber/Carbon Nanotube Nanocomposite with Hyperelastic Matrix

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**ABSTRACT**

An elastomer is a polymer with the property of viscoelasticity, generally having notably low Young's modulus and high yield strain compared with other materials. Elastomers, in particular rubbers, are used in a wide variety of products ranging from rubber hoses, isolation bearings, and shock absorbers to tires. Rubber has good properties and is thermal and electrical resistant. We used carbon nanotube in rubber and modeled this composite with ABAQUS software. Because of hyperelastic behavior of rubber we had to use a strain energy function for nanocomposites modeling. A sample of rubber was tested and gained uniaxial, biaxial and planar test data and then the data used to get a good strain energy function. Mooney-Rivlin form, Neo-Hookean form, Ogden form, Polynomial form, reduced polynomial form, Van der Waals form etc, are some methods to get strain function energy. Modulus of elasticity and Poisson ratio and some other mechanical properties gained for a representative volume element (RVE) of composite in this work. We also considered rubber as an elastic material and gained mechanical properties of composite and then compared result for elastic and hyperelastic rubber matrix together.



**Keywords:** Hyperelastic; RVE; Polynomial; Carbon nanotube

## 1 INTRODUCTION

A great deal of attention has been paid to tiny but fascinating carbon nanotubes (CNTs), which consist of rolled-up graphene sheet built from sp2 carbon units [1-3], because they are considered ideal reinforcing fillers in a wide range of composite systems [4]. This is due to their long macro-morphology (high aspect ratio, length/diameter) and their exceptional mechanical properties (Young's modulus=1-1.8 TPa) [5], transport conductivity and thermal conductivity (3000 W/m K) [6, 7]. Elastomers, in particular rubbers, are used in a wide variety of products ranging from rubber hoses, isolation bearings, shock absorbers to tires. Reinforcing the rubber with CNT makes a good composite with unique properties. Modeling of carbon nanotube composites has done in recent years for polymer matrix but in particular material such as rubber it has not been done completely. Rubber is a hyperelastic material and does not have constant mechanical properties. Then we should consider a good way to modeling rubber. The main goals of this work are:

- To understand the factors those need to be taken into consideration in order to model a rubber nano-composite;
- To create a suitable finite element representation for a RVE of an uniaxially reinforced nano-composite;
- To model a hyperelastic material and gain strain energy function of matrix.

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## 2 MODELING

For modeling it should be defined the properties of rubber. For hyperelastic material usually consider three test data [8, 9]. It suggests the data obtained under several stress states are preferred to optimise hyperelastic model predictions under multi-axial stress states [10]. Tests under uniaxial tension, biaxial tension and planar tension were performed. These tests are shown in Fig. 1. Three different est data are listed in Table 1 [11]. Strain energy function should be gained from these tests. Mooney-Rivlin form, Neo-Hookean form, Ogden form, Polynomial form, reduced polynomial form, Van der Waals form, etc., are some methods to get strain function energy [12, 13], that are shown in Fig. 2. With three test data, the best strain energy function is gained and then with ABAQUS software it can model RVE. By considering Table 1 and using the polynomial function, the elastic module and Poisson ratio of material obtained as follows [10]:

$$W = \sum_{i+j=1}^{N} C_{ij} (\bar{I}_B - 3)^i (\bar{I}_2 - 3)^j \quad (1)$$

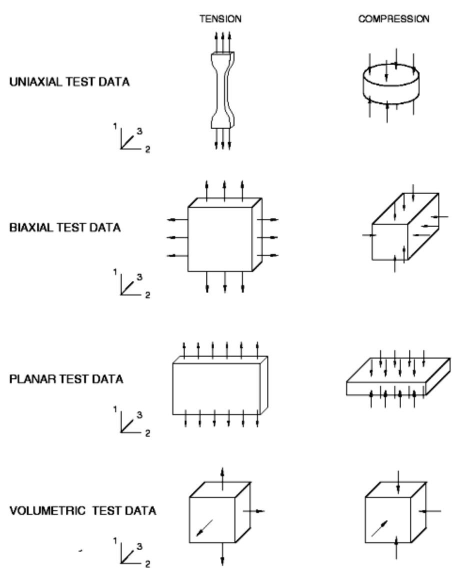


**Fig. 1**
Uniaxial, biaxial and planar tests for elastomers.

**Table 1**
Three test data for rubber

| Uniaxial test | | Biaxial test | | Planar test | |
|---|---|---|---|---|---|
| Stress (MPa) | Strain | Stress (MPa) | Strain | Stress (MPa) | Strain |
| 0.054 | 0.038 | 0.089 | 0.02 | 0.055 | 0.069 |
| 0.152 | 0.1338 | 0.255 | 0.14 | 0.324 | 0.2828 |
| 0.254 | 0.221 | 0.503 | 0.42 | 0.758 | 1.3862 |
| 0.362 | 0.345 | 0.958 | 1.49 | 1.269 | 3.0345 |
| 0.495 | 0.46 | 1.703 | 2.75 | 1.779 | 4.0621 |
| 0.583 | 0.6242 | 2.413 | 3.45 | - | - |
| 0.656 | 0.851 | - | - | - | - |

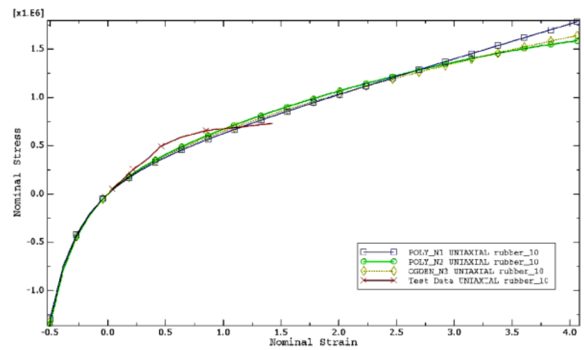


**Fig. 2**
Strain energy functions.

**Table 2**
Constants of Polynomial function

| | $D_1$ | $C_{10}$ | $C_{01}$ |
|---|---|---|---|
| polynomial | 0 | 176515.147 | 4302.5297 |

and

$$D_1 = \frac{3(1-2\nu)}{\mu_0(1+\nu)} \tag{2}$$

$D_1$, $C_{10}$ and $C_{01}$ are shown in Table 2. Because $D_1 = 0$ then from (2) the Poisson ratio will be $\nu = 0.5$ or in the other hand, the material is incompressible. At first, it assumed that rubber is a linear elastic material. It helps to simulate RVEs and obtain mechanical constants of nanocomposite. The mechanical properties of material are:

$$\begin{aligned} &\text{CNT} \rightarrow E = 1 \text{ (Tpa)}, \quad \nu = 0.3 \\ &\text{Rubber} \rightarrow E = 1 \text{ (Mpa)}, \quad \nu = 0.5 \end{aligned} \tag{3}$$

The properties of RVE are modeled as Liu & Chen [14].

$$\begin{aligned} &L = 100 \text{ ηm} \\ &R = 10 \text{ ηm} \\ &r_o = 5 \text{ ηm} \\ &r_i = 4.6 \text{ ηm} \end{aligned} \tag{4}$$

Continuum equations were used to estimate mechanical properties of nanocomposite. Three loads on RVE (Fig. 3) applied to gain four parameters: $\Delta L,\ \Delta R_a,\ \Delta R_b,\ \alpha$. They were obtained with FEM and substituted in continuum equation.

$$\begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix} = \begin{bmatrix} \frac{1}{E_x} & \frac{-\nu_{xy}}{E_x} & \frac{-\nu_{zx}}{E_z} \\ \frac{-\nu_{xy}}{E_x} & \frac{1}{E_y} & \frac{-\nu_{zx}}{E_z} \\ \frac{-\nu_{zx}}{E_z} & \frac{-\nu_{zx}}{E_z} & \frac{1}{E_z} \end{bmatrix} \begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{bmatrix} \tag{3}$$

In cylindrical RVE under an axial stretch (Fig. 3(a)), the stress and strain components at any point on the lateral surface are:

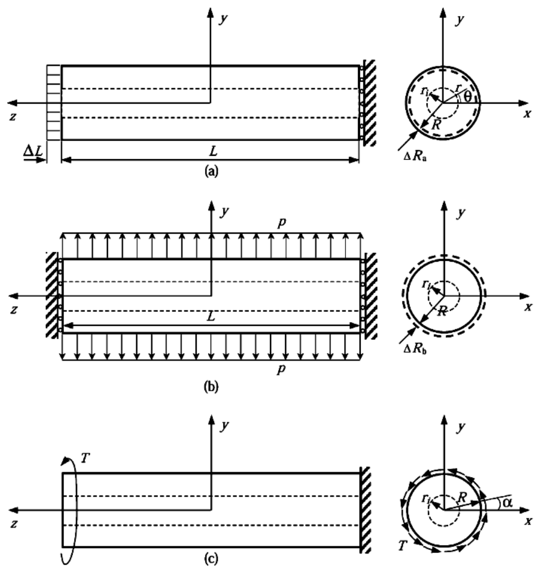


**Fig. 3**
Loads on RVE.

$$\sigma_x = \sigma_y = \sigma_r = \sigma_\theta = 0, \qquad \varepsilon_z = \frac{\Delta L}{L}, \qquad \varepsilon_\theta = \frac{\Delta R_a}{R}, \text{ with } \Delta R_a < 0 \text{ if } \Delta L > 0 \tag{4}$$

From the third equation in Eq. (3), one has immediately:

$$E_z = \frac{\sigma_z}{\varepsilon_z} = \frac{L}{\Delta L}\sigma_{ave} \tag{5}$$

$$\sigma_{ave} = \frac{1}{A}\int_A \sigma_z(x, y, L/2)\, \mathrm{d}x\, \mathrm{d}y \tag{6}$$

and

$$\nu_{zx} = -\frac{\Delta R_a}{R} / \frac{\Delta L}{L} \tag{7}$$

ABAQUS software is used to simulate RVE. Two types of element are used. Solid 8-node linear brick for CNTs and hybrid solid 8-node linear brick for rubber is used. The solid elements in ABAQUS are suitable for linear analysis and for complex non-linear analyses involving plasticity and large deformations. Hybrid elements are intended mainly for use with incompressible and almost incompressible materials. For a near incompressible material a very small change in displacement produces extremely large changes in pressure. Therefore, a purely displacement-based solution is too sensitive to be useful numerically. This singular behavior is removed by treating the pressure stress as an independently interpolated basic solution variable, coupled to the displacement. This independent interpolation of pressure stress is the basis of the hybrid elements. Hybrid elements have more internal variables than non-hybrid elements and this increase running time. Hybrid elements are recommended for hyperelastic materials. Square RVE also used in same method to obtain mechanical properties of nanocomposite and data are compared with “rule of mixture” in fiber composite materials [15]. For example, rule of mixture in square RVE is:

$$E_z = E_t V_t + E_m (1 - V_t) \tag{8}$$

where $E_t$ and $E_m$ are Young modules of carbon nanotube and matrix and $V_t$ is volume fraction of carbon nanotube that obtained by

$$V_t = \frac{\pi(r_0^2 - r_i^2)}{4a^2 - \pi r_i^2} \tag{9}$$

The notations are shown in Fig. 4.

## 3 RESULTS AND DISCUSSION

### *3.1 Mechanical properties*

Mechanical properties that obtained in RVE modeling are shown in Table 3. Results of simulation and theory of rule of mixture are nearly same. It means that simulations with selected elements are appropriate in this work. It is seen that the cylindrical RVE overestimates the Young's module. This may be explained by the fact that a cylindrical RVE overestimates the volume fraction of the CNT due to the negligence of the small amount of matrix material (at the four corners of the square RVE) in the cylindrical RVE.

### *3.2 Effect of change diameter of CNT on Young modulus*

Several diameters of CNT intend in this section. Thickness of CNT is constant and is 0.4 ηm. Fig. 5 shows the effect of diameter change on the Young modulus. As it's seen in Fig. 5, when the outer diameter of CNT increased, Young modulus of composite increased, too. It's because of increasing of volume fraction of CNT in nanocomposite.

### *3.3 Difference of modeling nonlinear elastic (hyperelastic) and linear elastic*

In previous sections, rubber was modeled as a linear elastic material. However, in reality, rubber is a hyperelastic (nonlinear elastic) material.

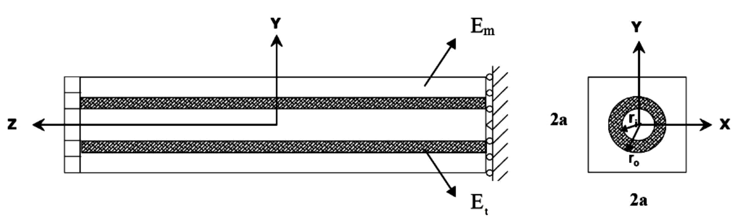


**Fig. 4**
Square RVE.

**Table 3**
Result of simulation of RVE

| RVE model | $E_z$, Simulation | $E_z$, Rule of mixture | $\nu_{zx}, \nu_{zy}$ | $E_x, E_y$ | $\nu_{xy}$ |
|---|---|---|---|---|---|
| Cylindrical | 48.96 (GPa) | 48 (GPa) | 0.4479 | 19.34 (MPa) | 0.573 |
| Square | 35.97 (GPa) | 36.17 (GPa) | 0.45 | 1.622 (MPa) | 0.4734 |

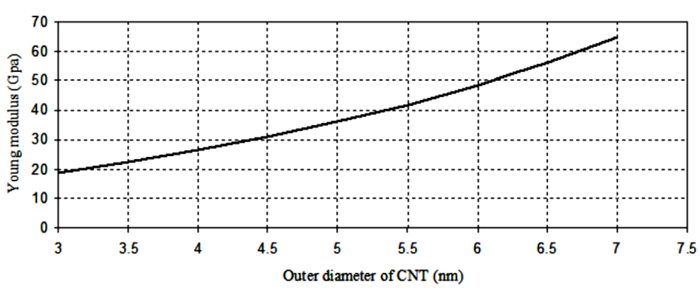


**Fig. 5**
Effect of diameter change on Young's module of composite.

Table 1 and Eq. (1) and (2) are used and hyperelastic material is modeled as a polynomial strain potential function. The stress-strain curve for polynomial function is shown in Fig. 6. For compare linear and nonlinear elastic rubber, two model with 25 CNT and rubber as a matrix are used (Fig. 7). In the first model, rubber is linear elastic and in the second model, rubber is nonlinear elastic. The difference between stress-strain curves for these two models is shown in Fig. 8.

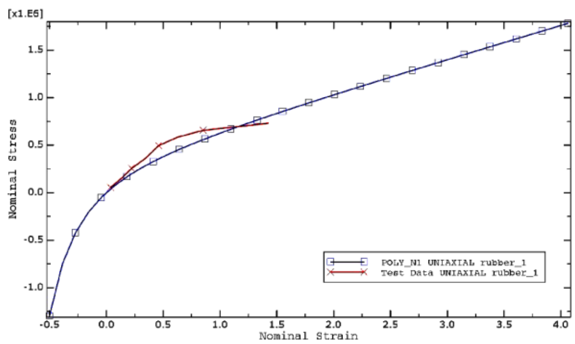


**Fig. 6**
Stress-strain curve for rubber with nonlinear elastic material.

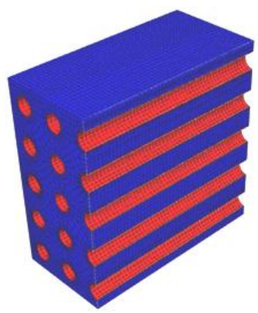

**Fig. 7**
Cut of composite model with 25 CNT.

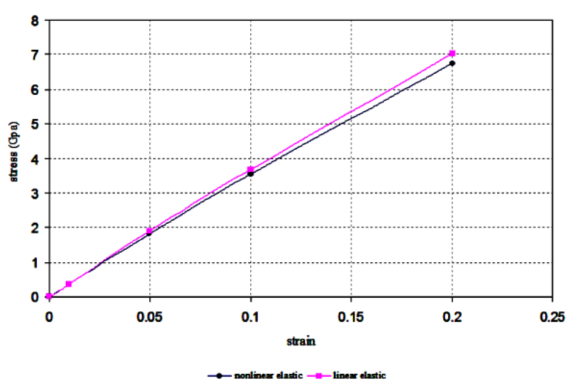


**Fig. 8**
Stress-strain curve of composite for linear and nonlinear elastic rubber.

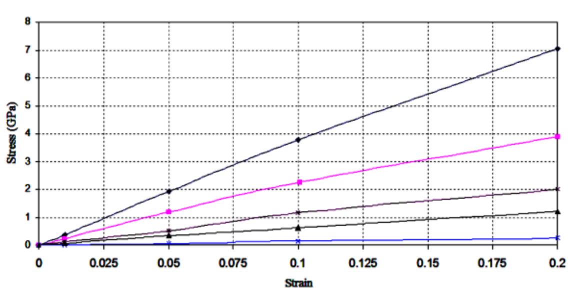


**Fig. 9**
Stress-strain curve of composite several percent of volume fraction of CNT in rubber.

As it seen in Fig. 8 difference between two curves increases by strain increases. It's because of assumption linear or nonlinear elastic rubber. Linear elastic assumption of rubber is correct only for low strain.

### *3.4 Volume fraction*

The effect of volume fraction of CNT in rubber also was modeled. Several percent of volume fraction was intended. 0.12%, 0.628%, 1.16%, 2.05% and 3.75% of volume fraction of CNT in rubber was modeled and the stress-strain curves for them were depicted. Fig. 9 shows this modeling.

## 4 CONCLSIONS

Rubber was reinforced with CNTs in this work. At first, rubber was considered as a linear elastic material and with finite element analysis, mechanical properties of nanocomposite were gained. Then, rubber was modeled as a hyperelastic material with polynomial strain energy function and the behavior of nanocomposite here was studied. It saw that linear elastic assumption of rubber is correct only for low strain and for large strain rubber should be modeled as a hyperelastic material. Furthermore, several volume fractions of carbon nanotubes in rubber were modeled and it was shown that stiffness of nanocomposite was increased by more volume fraction of CNTs. We considered rubber as a hyperelastic material and gained Young's module and Poisson ratio in three surfaces. Then test data assumed linear and we supposed to $E$=1 MPa and this time RVE is considered as an elastic and incompressible material. Elastic modulus gained with continuum equating and strain matrix.

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