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A Numerical Evaluation of The Deformation of a Polymer Matrix Caused by Change in Orientation of Embeded Carbon Nanotubes Under an Electric Field

KEYWORDS: Carbon nanotubes, electric field, orientation, strain, polymeric matrix, inclusions, stress, polymers, conductors and polyethylene.

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ABSTRACT *Polymers that act under the action of an electric current have become an area of interest in the development of artificial muscles, control systems, medical devices, amongst others. In addition carbon nanotubes (CNT) are an excellent option to these purposes because possess excellent mechanical and electrical properties, that can add stiffness and electrical conductivity to polymers. Despite numerous studies on carbon nanotubes, very few research can be found on the deformation of polymeric matrices caused by the orientation of carbon nanotubes under the of action an electric field, so in this research a first approach to the deformation of a polyethylene matrix with inclusions of CNT is presented. To achieve this deformation, the orientation of the CNT was simulated by the finite element method in which an electric field is generated by applying a potential difference of 10 volts (from -5 to 5 volts on two conductors) which generate an electric field E 8.033x10-7 = V /m. The electric field in turn generates a moment and a polarization of the nanotubes so that these are aligned vertically. The maximum deformation were obtained in the polyethylene matrix where the inclusions of carbon nanotubes, while every stress was obtained in carbon nanotubes*

1 Introduction

A carbon nanotube (CNT) possesses very elongated structure, and are capable to reacting to the action of an electrical field. This interaction of the electric field with carbon nanotubes have different effects, some of these effects is related to promoting the orientation of the nanotubes in different means. Another effect of the electrical field can be related to the contact potential difference between the nanotube and the material. All these effects call for a more detailed theoretical and experimental study of the influence of the electric field on the alignment of CNTs. For example Tang et al [1] determine that an electric field E induces a dipole moment in a neutral particle and this interaction potential of two neutral particles at large distances from each other is determined by the values of these induced dipole moments.

Other investigations have reported the orientation of carbón nanotubes, so in the table 1 different methods CNTs orientatiton shown.

Table 1. Orientation methods

Method	Author
Spinning of CNTs	Ericson, 2004 [2]
Condensing of viscous flow-aligned polymer-CNT composites	Vigolo et al [3]
Applying electrical field	Kamat et al [4] Takahashi et al [5]
Using the cooperative reorientation of a liquid-crystal-CNT suspensión in electric field	Dierking et al [6]
Magnetic orientation of CNTs using srong magnetic field	Fujiwara et al [7] Kawakami et al [8] Fischer et al [9] Zaric et al [10].

Carbon nanotubes (CNTs) have unique emission characteristics [11-15] which are caused by their high aspect ratio and good electrical conductivity. In combination with high termal, mechanical and chemical stability, these properties of CNTs determine a possibility of development of a new type of vacuum electronic devices, CNT-based electron field emission cathodes. In contrast with conventional electron field emitters, such cathodes operate at a relatively low applied voltage (at level 1 kV), which allows the development of miniature devices. This is caused by the enhancement of the electrical field, mainly because of it is effect near a nanotube tip which can be several hundred times higher than the average electric field strength in the interelectrode gap. A wide application of CNT-based cathodes and the prospects of their use in flat monitors [16-18] X-ray sources [19-27], lighting tubes [28-33], and microwave radiation generators and amplifiers involved in the systems of space communication [34-35] make it necessary to find the physical factors that limit the emission current density from such cathodes and determine the máximum posible current density.

Since the discovery of single-walled carbon nanotubes

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(SWNTs), they have been expected to become the building blocks of to next generation functional nanomaterials. However, their strong cohesive property and poor solubility have been restricted their application to fundamental and applied research fields. One of the methods to overcom these problems is place the SWNTs soluble in solvents and wrapping them with polymers [36]. At the same time, the fabrication of high-performance carbon-nanotube (CNT)-based composites is driven by the ability to create anisotropy at the molecular level to obtain desired properties

2 Alignment of carbon nanotubes under the action of an electric field

As described by alignment of carbon nanotubes [38] can be achieved when the angle of orientation relative to the nanotube material depends on the strength of the external electric field directed perpendicular to the plane of the material

Therefore, a problem arises in dependence on the angle of orientation of carbon nanotube material with respect to the electric field.

The value of this angle can be determined from the mechanical balance of the forces acting on the nanotube. Electric field *E* induces a polarization *P* of charges in the conducting nanotube, equal to $P = \alpha_{\parallel} E\cos\phi$. Here, $\alpha_{\parallel}$ is the longitudinal polarizability of the tube. The interaction between the electric dipole formed in such a way and the electric field generates moment *M* [37-38], which is expressed by:

$$M = E = \frac{1}{2}E^2(\alpha_{II} - \alpha_{\perp})\sin(2\varphi) \quad (1)$$

According to numerical computations [39], the longitudinal and transverse polarizability of the CNTs are:

$$\alpha_{II} = (0.23 + 0.135D)(L^2 + 52.5) \quad (2)$$

$$\alpha_{\perp} = (0.12D^2 + 1.76)(L + 4.65) \quad (3)$$

where *D* and *L* are the diameter and length of the nanotube respectively. The longitudinal polarizability is approximately *L/D* times higher than the transverse polarizability and for the nanotubes with large aspect ratio *L/D* >> 1, the transverse polarizability is negligibly as compared to the longitudinal polarizability.
For a single-layer of CNT, $D^4 - d^4 \approx 4\delta D^3$, where δ is the effective thickness of the nanotube wall and is approximately 3.4 Å. The angle of CNT bending under the action of the electric field is determined from the equation of mechanical balance between the bending moment and the moment of elastic forces, such that:

$$E^2(\alpha_{II} - \alpha_{\perp})\sin(2\varphi)/2 = 0.5\frac{Y(D^4 - d^4)}{L}(\theta - \varphi) \quad (4)$$

where the angle $\theta - \phi$ is the CNT bending angle. Equation (4) permits the estimation of the value of electric field strength *Ec*, which compensates the initial bending of the nanotube. Taking into account the condition $\phi << 1$ then:

$$E^2 = Y\frac{(D^4 - d^4)}{L^3 D} \quad (5)$$

In the case of a multilayer CNT, the Equation (5) is reduced to:

$$E^2 = Y\left(\frac{D}{L}\right)^3 \quad (6)$$

while in the case of a single-layer CNT, one can write:

$$E^2 = Y\frac{4\delta}{D}\left(\frac{D}{L}\right)^3 \quad (7)$$

3 Methodology and finite element analysis

The material used for this research is a high molecular weight polyethylene which is used as the matrix, the properties of this material is shown in Table 2.

Table 2. Properties of Polyethylene

High Molecular Weight Polyethylene	
Density	950 Kg/m^3
Modulus of elasticity	.565 – 1.50 GPa
Poisson	.42
Yield stress to strain	11 – 43 MPa
Yield stress compressive	4 – 31.7 Mpa
Ultimate tensile strength	10 – 43 Mpa
Ultimate compressive strength	4 - 31.7 MPa
Electrical Resistivity	1 x 10^{16} Ωm

Carbon nanotubes are added within the polyethylene matrix. Table 3 shows properties of carbon nanotubes.

Table 3. Properties of carbon nanotubes

Properties of carbon nanotubes	
Density	1400 Kg/m^3
Modulus of elasticity	.6 TPa
Ultimate strength	200 MPa
Hardness	200 GPa
Surface energy	8.53 J/m^2
Poisson	.186
Electrical Resistivity	1 x 10^{-6}

The geometry is made for analysis is very simple, in order to check that there is deformation in the polyethylene matrix because of the orientation of the carbon nanotubes generated by an electric field. The matrix of polyethylene has a diameter of 500 microns and a length of 550 microns, meanwhile carbon nanotubes have a diameter of 5 microns and a length of 100 microns, and the gap that exists between the nanotubes is longitudinally 50 microns. This is shown in Figure 1a, and 204 carbon nanotubes that percentage is 26.3% were used.

To generate the electric field are two conductors within the matrix, this conductors have a diameter of 20 microns and a length of 550 microns were used.The conductors we applied a voltage of 5 volts and -5 respectively to generate an electric field E = 8.033x10-7 V / m on carbon nanotubes, according to the electric analysis. In Figure 1b shown the electrical analysis where the force vectors of the conductors emerging because of the applied voltage which in turn generates the electric field E = 2.4x107 observed on the conductive.

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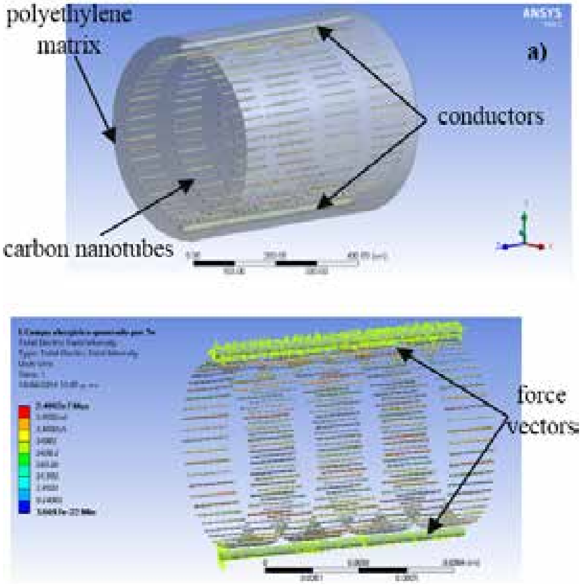

Figure 1. a) Geometry of the model for analysis and b) electric field generated in the electrical analysis by conductive.

The model has a total of 1359301 nodes and 597319 elements, the meshing was held with elements of tetrahedral type, Figure 2a shows the meshing in the matrix and in Figure 2b shows the mesh in carbon nanotubes. It is observed that the mesh is much finer in the area where the carbon nanotubes, this is caused by the change in geometry between the matrix and these nanotubes.

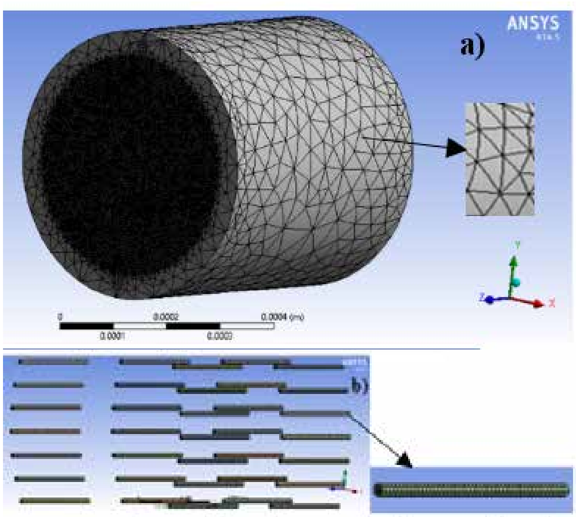

Figure 2.a) Meshing the matrix b) Meshing in carbon nanotubes.

The electric field direction is from the conductive of the 5 volt to -5 volt with conductive, therefore the nanotube is oriented to said address, to show that, in figure 3 the direction of the electric field is shown, it is noteworthy lines presented pass on carbon nanotubes.

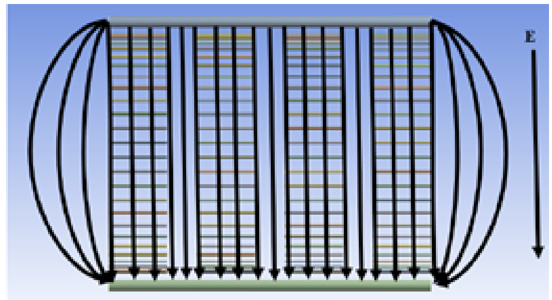

Figure 3. Direction of the electric field.

According Equation 1 to generate the moment M over the nanotubes is necessary to determine both the electric field and the dipole moment being generated by the field, therefore the electrical analysis was performed to obtain the field acting on the nanotubes shown in Figure 1a. However, once calculated the electric field is necessary to calculate the polarization longitudinal and transverse using equation 2 and 3. To obtain these values we can calculate the moment M is the force exerted on carbon nanotubes in the static analysis and because the electric field according to Faraday's constant force on the nanotubes is the same in each nanotubes. In Table 4, the boundary conditions were used according to the calculations for the model being analyzed are presented.

Table 4. Boundary conditions

Condition	Value
Voltage on the conductors	5 and -5 Volts
Polarization longitudinal	12.075 $Å^3$
Polarization transverse	8.184 $Å^3$
Moment	1.25×10^{-12} N

The electrical analysis show apart from the electric field generated, also shows another important aspect as the heat generated due to the voltage applied on the conductor. This is important because you have to remember that the polymer needle is inserted on the patient and if too much heat is generated that could generate discomfort. The maximum heat generated is had on the conductor (as shown in Figure 4) to which 5 volts is applied with a value of 1403 W / m3 which is minimal and the heat generated on the array is even smaller.

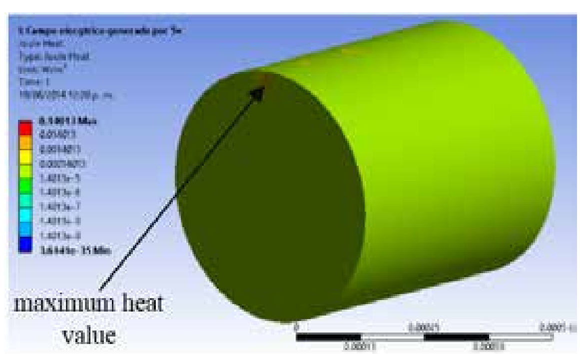

Figure 4. The maximum heat is generated on the conductor.

With M = 1.25×10^{-13} the moment for both the static deformation of the matrix because of the carbon nanotubes

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and the orientation of the latter analysis is performed. As mentioned above the force exerted on each of the carbon nanotubes as shown in Figure 5.

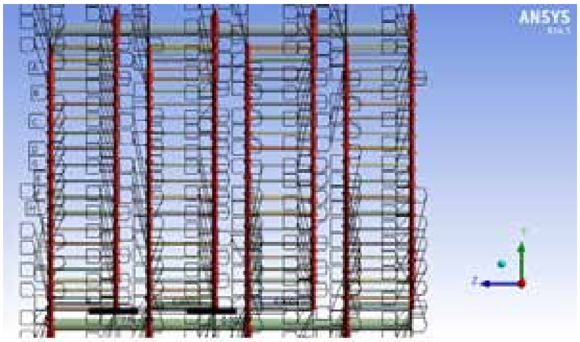
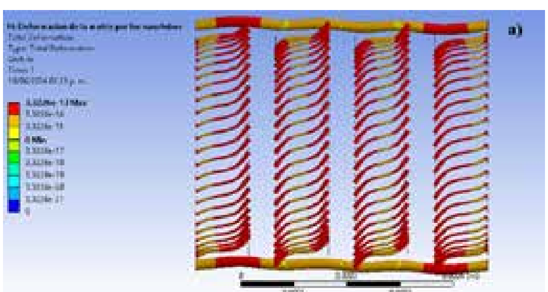
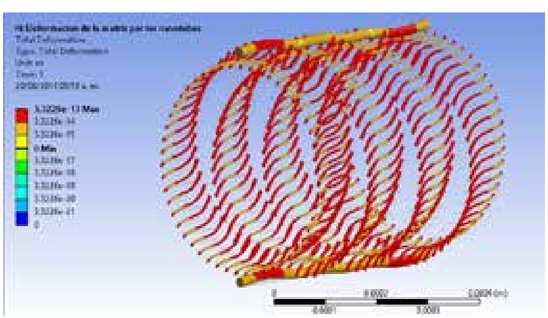
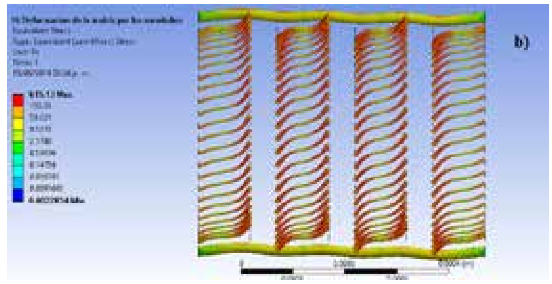


Figure 5. Distribution of the forces on the nanotube.

By exerting the force on the nanotubes, this causes the nanotubes are oriented in the direction of the electric field, causing the deformation of the polyethylene matrix moreover maximum stress are found in nanotubes because of their high modulus of elasticity than polyethylene. In Figure 6 the orientation obtained carbon nanotubes and stress generated about them is displayed, an important aspect to note is that apparently the nanotubes exhibit a deformation which is not correct because the force applied is too small compared to the elastic modulus of the nanotubes, we observe that there is deformation since the program exaggerates infinite element deformations in order to appreciate the behavior of the phenomenon, that is why it must be clarified that the nanotubes do not exhibit no deformation, but if possible orientation as seen while the deformations are very small.







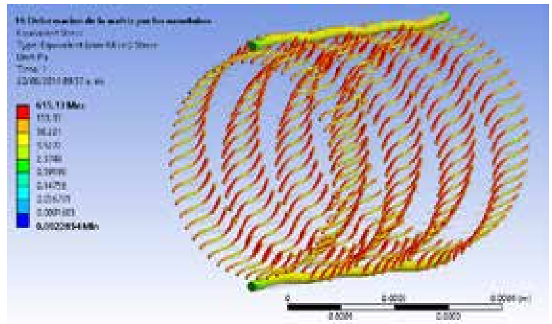


Figure 6. a) Orientation of carbón nanotubes and b) Stress generated on nanotubes.

As mentioned above the deformation that occurs in the matrix is generated by the approach outlined in the carbon nanotubes, such deformation of the matrix is approximately 3.226×10^{-13} m, the greatest deformation where they are positioned are carbon nanotubes as shown in Figure 7, and the smaller stresses are in those areas where there is no presence of nanotubes. As stress as mentioned are given in the carbon nanotubes as shown in Figure 8.

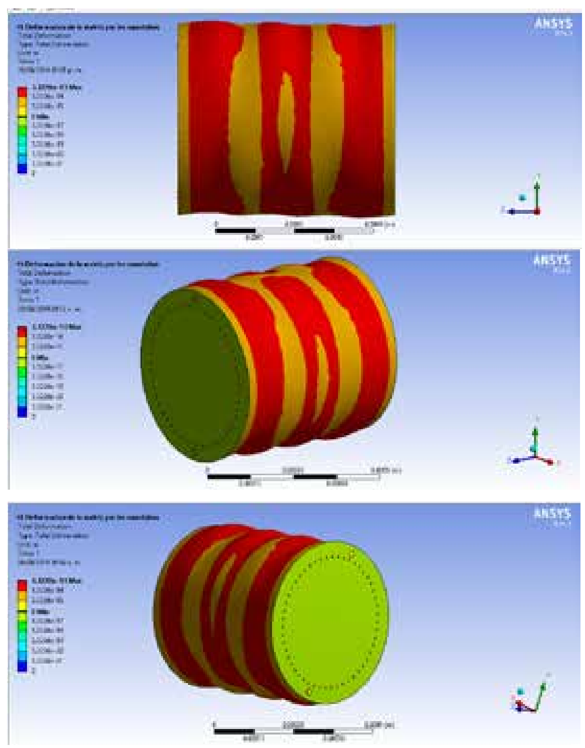


Figure 7. Deformation polyethylene matrix

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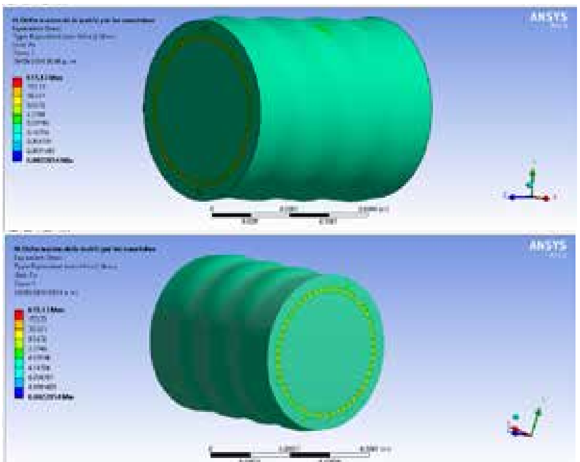

Figure 8. The maximum stresses are in carbon nanotubes.

4 Discussion

With $3.5x10^{-8}$ conductor area and an applied voltage of 5 volts, an electric field E = E = $8.033x10^{-7}$ V / m is generated, if the area of the conductor increases the electric field also increase because the field is a function of the area and thus the force applied to the nanotubes will be greater and greater strain on this matrix will polyethylene. With the force generated from the electric field and the polarization of the nanotubes one has a displacement or deformation of the matrix $3.226x^{-13}$ m, this deformation would seem that very little, however, consider that the area of $1.25x10^{-6}$ matrix is taking this into account the deformation generated by carbon nanotubes is not a insignificant. By applying the force on nanotubes that this generates maximum stresses occur in these with a value of about 615 Pa.

5 Conclusions

According to the analysis presented can be targeted carbon nanotubes in a polyethylene matrix. This can be accomplished after generation of an electric field inducing a voltage two conductors 5 and -5 volts, the electric field in turn generates a force and a polarization of the nanotubes which result in the creation of a moment on the nanotubes. As presented in this analysis is possible to deform the matrix with the orientation of carbon nanotubes and although the deformations obtained on the matrix are relatively small the amount is the phenomenon that was achieved and the importance of this analysis and that this could if possible the enervation of polymeric needle. Moreover, the force generated can be increased with the voltage applied on the conductor and if the voltage is increased accordingly if increase the electric field and in turn the force applied to the nanotubes for orientation. Furthermore, if the percentage of carbon nanotubes increases the deformation in the matrix will be greater.

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