

EVALUATION OF THE DEFORMATION OF A POLYMER MATRIX CAUSED BY THE CHANGE IN THE ORIENTATION OF EMBEDDED CARBON NANOTUBES UNDER AN ELECTRIC FIELD

EVALUATION OF THE DEFORMATION OF A POLYMER MATRIX CAUSED BY THE CHANGE IN THE ORIENTATION OF EMBEDDED CARBON NANOTUBES UNDER AN ELECTRIC FIELD

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Abstract – Electroactive polymers (EAPs) have become an area of interest for the development of artificial muscles, control systems, medical devices, among others. Additionally, carbon nanotubes (CNTs) are an excellent option for these purposes because they have excellent mechanical and electrical properties, which can add rigidity and electrical conductivity to polymers. Although there are numerous studies on CNTs, very few of them address the deformation of polymer matrices caused by the orientation of these CNTs under the action of an electric field. Therefore, this research presents a first approximation of the deformation of a polyethylene matrix with CNT inclusions. To achieve this deformation, the orientation of the CNTs was simulated using the finite element method, in which an electric field is generated by applying a potential difference of 10 volts (from -5 to 5 volts in two conductors) that generates an electric field $E = 8.033 \times 10^{(-7)} \text{ V/m}$. The

electric field in turn generates a torque and a polarization on the nanotubes, causing them to align vertically. The results showed that the polyethylene matrix exhibited greater deformation in the regions where the CNT inclusions are located, while the highest stress concentrations occurred in the CNTs themselves.

Keywords: Electric field, Mechanical deformation, Polymer matrix, Finite element method, Carbon nanotubes (CNT), Electroactive polymers (EAP).

Abstract – Electroactive polymers have gained significant interest in fields such as the development of artificial muscles, control systems, medical devices, and more. Additionally, carbon nanotubes (CNT) are an excellent option for these purposes because they possess outstanding mechanical and electrical properties, which can enhance the rigidity and electrical conductivity of polymers. However, despite extensive studies on CNT, very few of them have addressed the deformation of polymeric matrices caused by the orientation of CNT under the influence of an electric field. Therefore, this work presents a preliminary approach to the deformation of a polyethylene matrix with CNT inclusions.

To achieve this deformation, the orientation of the CNT was simulated using the finite element method, where an electric field was generated by applying a potential difference of 10 volts (ranging from -5 to 5 volts across two conductors), resulting in an electric field $E = 8.033 \times 10^{(-7)} \text{ V/m}$. The electric field, in turn, induces a moment and polarization on the nanotubes, causing them to align vertically. The results showed that the polyethylene matrix exhibited the highest deformation in regions with CNT inclusions, while the highest stress concentrations occurred within the nanotubes themselves.

Key words – Electric field, Mechanical deformation, Polymeric matrix, Finite element method, Carbon nanotubes (CNT), electroactive polymers (EAP).

INTRODUCTION

Carbon nanotubes (CNTs) have an elongated structure and are capable of reacting to the action of an

electric field. This interaction between the electric field and CNTs has different effects, one of which is related to promoting the orientation of nanotubes in different media. Another effect of the electric field is related to the difference in contact potential between the nanotube and the material. A more in-depth theoretical and experimental study of the influence of the electric field on the alignment of CNTs is necessary. For example, Tang and Liang [1] determine that the electric field E induces a dipole moment in a neutral particle and this interaction potential of two neutral particles in great distances from each other is determined by the values of these induced dipole moments.

CNTs have unique emission characteristics [2-6], which are caused by their high aspect ratio and good electrical conductivity. In combination with high thermal, mechanical, and chemical stability, these properties of CNTs determine the possibility of developing a new type of vacuum electronic device involving electron fields on

CNT-based emission cathodes. In contrast to conventional electron field emitters, cathodes operate at a relatively low applied voltage (at the 1 kV level), which allows for the development of miniature devices. This is caused by the enhancement of the electric field, mainly due to the effect near a nanotube tip, which can be several hundred times greater than the average electric field strength in the space between the electrodes. There is a wide application of CNT-based cathodes and prospects for their use in flat monitors [7], X-ray sources [8-14], lighting tubes [15-18], and generators and amplifiers involved in microwave radiation [19,20] make it necessary to find the physical factors that limit the emission current density of such cathodes to determine the maximum possible current density.

Since the discovery of single-walled carbon nanotubes (SWCNTs), they have been expected to be the building blocks of a new generation of functional nanomaterials. However, their strong cohesive properties and poor solubility have restricted their application to fundamental and applied research fields. One of the methods to overcome these problems is to coat SWCNTs with polymers. In turn, the efficient manufacture of composites with CNTs is driven by the ability to create anisotropy at the molecular level to obtain the desired properties [21].

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

The alignment of CNTs, according to M.A. Shao-Jie [22], can be achieved when the angle of the nanotube relative to the material depends of the strength of the external electric field directed perpendicular to the plane of said material. Therefore

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

The value of this angle can be determined from the mechanical equilibrium of the forces acting on the nanotube. The electric field E induces polarization P in the conductive nanotube, $P = \alpha_{II} E \cos(\varphi)$. Here, α_{II} is the longitudinal polarizability of the tube. The interaction between the electric dipole formed and the electric field generates a moment M [22,23], which is expressed by:

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

According to numerical calculations [22-23], the longitudinal and transverse polarizability of 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 nanotubes with a large aspect ratio $L/D \gg 1$, the transverse polarizability is negligible compared to the longitudinal polarizability.

For a single layer of CNTs, $D^4 - D^4 \approx 4\delta D^3$, where δ is the effective wall thickness of the nanotubes and is approximately 3.4 nanometers. The bending angle of CNTs under the action of the electric field is determined from the mechanical equilibrium equation between the bending moment and the moment of elastic forces, such that:

$$E^2 (\alpha_{II} - \alpha_{\perp}) \sin(2\varphi) / 2 = 0.15 \frac{Y(D^4 - d^4)}{L} (\theta - \varphi) \quad (4)$$

where the angle $\theta - \varphi$ is the bending angle of the nanotube. Equation (5) allows the estimation of the value of the electric field intensity E_C , which compensates for the initial bending of the nanotube. Taking into account the condition $\varphi \ll 1$, then:

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

In the case of a multi-walled CNT, 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, it can be written as:

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

DEVELOPMENT METHODOLOGY AND FINITE ELEMENT ANALYSIS

The material used for this research is high molecular weight polyethylene, which is used as a matrix. The properties of this material are shown in Table 1.

Carbon nanotubes are added to the polyethylene matrix in the form of inclusions. Table 2 shows the properties of carbon nanotubes.

Table 1. Properties of polyethylene.

High molecular weight polyethylene	
Density	950 kg/m ³
Modulus of elasticity	0.565 – 1.50 GPa
Poisson's ratio	0.42
Yield strength	11 – 43 MPa
Yield strength under compression	4 – 31.7 MPa
Ultimate tensile stress	10 – 43 MPa
Ultimate compressive stress	4 - 31.7 MPa
Electrical resistivity	1 x 10 ¹⁶ Ωm

Source: Mechanical properties of polyethylene (Zully Vargas Galarza, 2025).

Table 2. Properties of carbon nanotubes.

Properties of carbon nanotubes	
Density	1400 kg/m ³
Modulus of elasticity	0.6 TPa
Ultimate stress	200 MPa
Hardness	200 GPa
Surface energy	8.53 J/m ²
Poisson's ratio	0.186
Electrical resistivity	1 x 10 ⁻⁶ Ωm

Source: Mechanical properties of single-walled carbon nanotubes (Porfirio Roberto Nájera Medina, 2025).

The geometry used for the analysis is quite simple, with the aim of verifying the deformation that exists in the polyethylene matrix due to the orientation of the CNTs generated by an electric field. The polyethylene matrix has a diameter of 500 microns and a length of 550 microns, while the carbon nanotubes have a diameter of 5 microns and a length of 100 microns, and the longitudinal separation between the nanotubes is 50 microns. This is shown in Figure 1a. A total of 204 CNTs were used, representing 26.3% of the polyethylene matrix.

To generate the electric field, two conductors located within the matrix were used. These

CITID 2025 ISSN: 2594-2905 have a diameter of 20 microns and a length of 550 microns. A voltage of 5 and -5 volts was applied to the conductors, respectively, to generate an electric field $E = 8.033 \times 10^{-7} \text{V/m}$ over the carbon nanotubes, according to the electrical analysis.

Figure 1b shows the electrical analysis, where the force vectors emerging from the conductors due to the applied voltage can be observed, which in turn generate the electric field $E = 2.4 \times 10^{-7} \text{V/m}$ on the conductor.

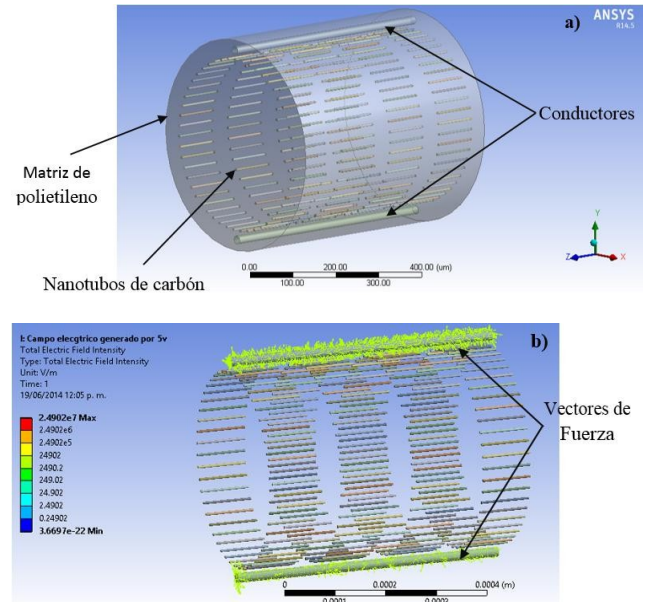
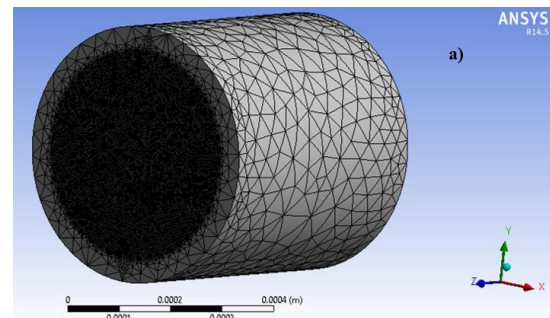


Figure 1. a) Geometry of the model for analysis and b) Electric field generated in the electrical analysis by the conductors (Zully Vargas Galarza, 2025).

The model has a total of 1,359,301 nodes and 597,319 elements. The mesh was created using tetrahedral elements. Figure 2a shows the mesh in the matrix, and Figure 2b shows the mesh in the CNTs. It can be seen that the mesh is much finer in the area where the carbon nanotubes are located. This is caused by the change in geometry between the matrix and the nanotubes.



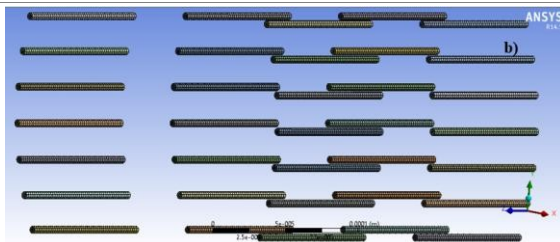


Figure 2. a) Mesh in the matrix and b) Mesh in the carbon nanotubes (Enrique López Chávez, 2025).

The direction of the electric field is from the 5-volt conductor to the -5-volt conductor, which is why the nanotubes are oriented in that direction. To illustrate this, Figure 3 shows the direction of the electric field. It should be noted that the lines shown pass over the carbon nanotubes.

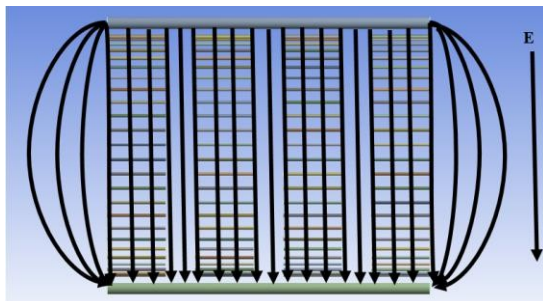


Figure 3. Direction of the electric field (José Efraín Ruíz Ramírez, 2025).

According to equation (1), to generate the moment M on the nanotubes, it is necessary to calculate both the electric field and the dipole moment that generates said field. For this reason, an electrical analysis was performed to obtain the field acting on the nanotubes shown in Figure 1b. Now, once the electric field has been calculated, it is necessary to calculate the longitudinal and transverse polarization using equations 2 and 3. Once these values are obtained, it is possible to calculate the moment M , which is the force acting on the carbon nanotubes in the static analysis. Since the electric field is constant according to Faraday, the force on the nanotubes is the same in each of the nanotubes. Table 3 shows the boundary conditions that were used according to the calculations for the model being analyzed.

Table 3. Boundary conditions.

Condition	Value
Voltage across the conductors	5 and -5 Volts
Longitudinal polarization	$12.075 \text{ \AA}^3$
Transverse polarization	$8.184 \text{ \AA}^3$
Moment	$1.25 \times 10^{-12} \text{ N}$

Source: Boundary conditions applied to the model (José Aldo Salazar Neri, 2025).

25 ISSN: 2594-2905 to showing the electric field that is generated, the electrical analysis also shows another important aspect, such as the heat generated by the voltage applied to the conductors. This point is important because it must be remembered that the polymer needle is inserted into the patient and if too much heat is generated, this could cause discomfort. The maximum heat value is concentrated in the conductor (as shown in Figure 4) to which 5 volts are applied with a value of 0.1403 W/m^3 which is minimal, and the heat generated on the matrix is even lower.

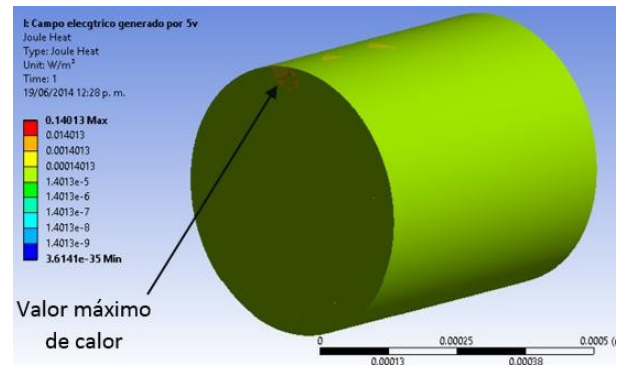


Figure 4. The maximum heat is generated on the conductor (José Efraín Ruíz Ramírez, 2025).

With the moment $M = 1.25 \times 10^{-13} \text{ Nm}$, the static analysis is performed to obtain both the deformation of the matrix caused by the CNTs and the orientation of the latter. As mentioned above, the force is exerted on each of the carbon nanotubes as shown in Figure 5.

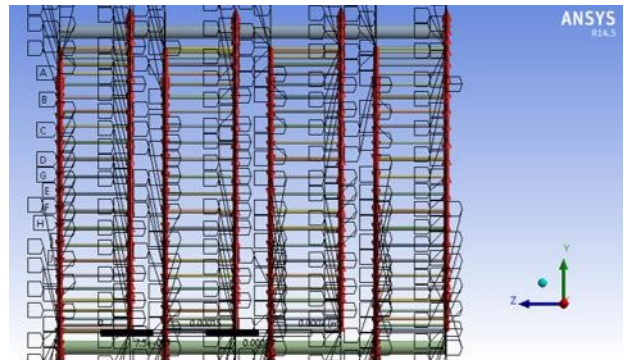


Figure 5. Distribution of forces on the nanotubes (Porfirio Roberto Nájera Medina, 2025).

When force is exerted on the nanotubes, they orient themselves in the direction of the electric field, causing deformation of the polyethylene matrix. On the other hand, the highest stress concentrations occurred in the nanotubes themselves due to their high modulus of elasticity compared to polyethylene. Figure 6 shows the orientation of the CNTs and the stresses generated on them. It is important to note that the nanotubes appear to be deformed, which is not

correct, since the force applied is too small compared to the stress concentrations are found in areas where there are no nanotubes. As mentioned, the stresses are concentrated in the carbon nanotubes, as shown in Figure 8.

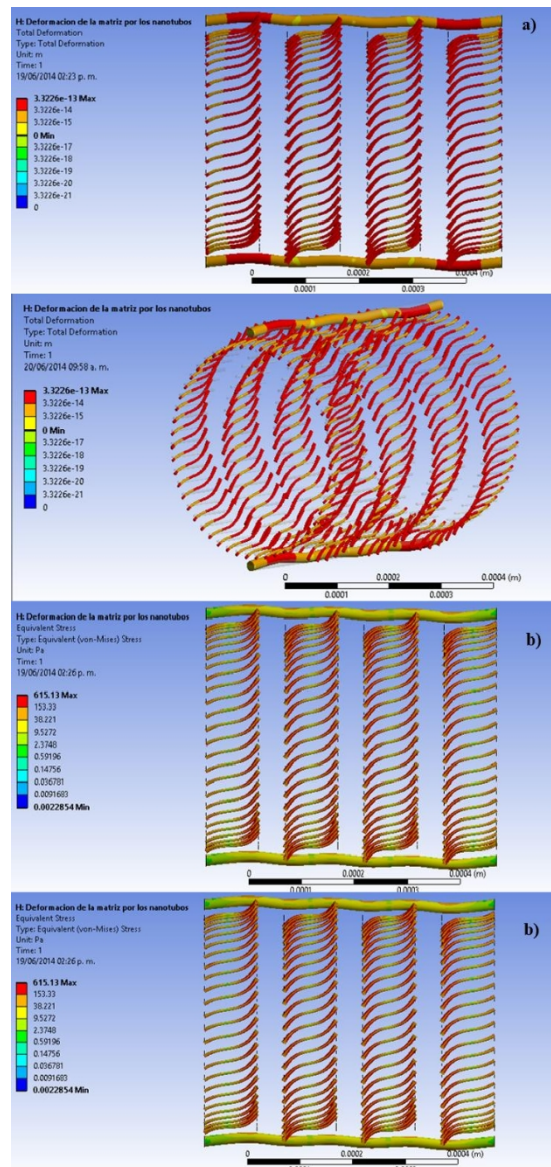


Figure 6. a) Orientation of carbon nanotubes and b) Forces generated on nanotubes (Enrique López Chávez, 2025).

As mentioned above, the deformation that occurs in the matrix is generated by the orientation of the CNTs. This deformation of the matrix is approximately 3.226×10^{-13} m, and greater deformation occurred in the regions where CNT inclusions are found, as shown in Figure 7.

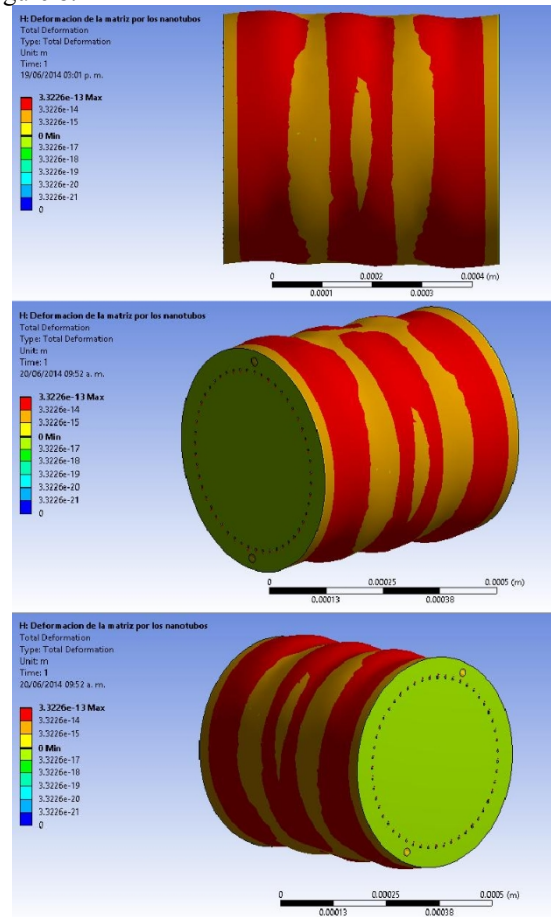


Figure 7. Deformation of the polyethylene matrix (Enrique López Chávez, 2025)

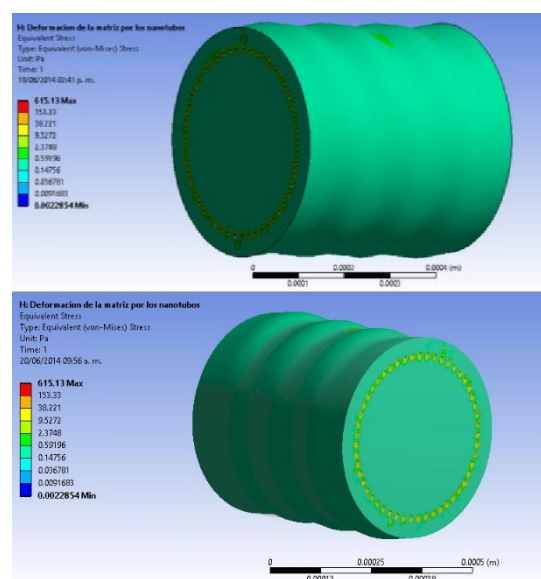


Figure 8. Maximum stresses are found in carbon nanotubes (José Aldo Salazar Neri, 2025).

DISCUSSION AND ANALYSIS OF RESULTS

With a conductor area of $3.5 \times 10^{-8} m^2$ and an applied voltage of 5 volts, an electric field $E = 8.033 \times 10^{-7} V/m$ is generated. If the conductor area increases, the electric field will also increase since the field is a function of the area and, consequently, the force applied to the nanotubes will be greater, causing greater deformation of the polyethylene matrix. With the force generated by the electric field and the polarization on the nanotubes, there is a displacement or deformation of the matrix equal to $3.226 \times 10^{-13} m$. Although this value may seem small, considering that the area of the matrix is $1.25 \times 10^{-6} m^2$, the deformation induced by the CNTs becomes more significant. The application of force on the nanotubes generates a maximum concentration of forces on them, with an approximate value of 615 Pa.

Effect of the electric field on the orientation and deformation of CNTs:

According to Baughman et al. (2002) in their study on nanotube-based actuators [24], it is established that the application of electric fields generates induced polarization in CNTs, causing tensile or compressive forces that can be transmitted to the polymer matrix through the interface. Although the linear deformation may be small, the cumulative effects at the macro scale can result in measurable changes in the shape, elastic modulus, or stress direction of the composite material.

Relationship between the cross-sectional area of the conductor and the increase in the effective field:

The approach suggests that increasing the conductor area also increases the electric field. However, from a physical point of view, the electric field ($E = V/d$) is independent of area and depends directly on the voltage and distance between electrodes. Nevertheless, the current flow or induced charge density does depend on area, which could increase the net force acting on the CNTs.

Studies such as that by Tavakkol et al. (2014) show how an increase in CNT density or in the efficiency of the CNT-matrix contact leads to greater transmission of the force induced by the electric field, especially in matrices such as polyethylene. This translates into greater local deformations [25].

Stress concentration and its effect on the matrix:

The maximum stress concentration of 615 Pa observed in CNTs represents a moderate value, but not negligible considering the nanometric scales. In fact, Li and Chou (2003) demonstrated that in CNT-reinforced nanocomposites reinforced with CNTs, even very small forces can induce significant localized deformations, altering the overall properties of the material. This is

due to the high surface-to-volume ratio of nanotubes and their efficiency in transferring mechanical loads [26].

CONCLUSIONS

The result shows how the generated electric field influences the deformation of the polyethylene matrix. As the conductor area increases, the electric field increases and, consequently, the force on the carbon nanotubes (CNTs) also increases, leading to greater deformation. This concept is important because it suggests a direct relationship between the conductor area and the deformation induced in the matrix, allowing for controlled manipulation of the deformation by adjusting the area. Although the deformation may appear small, the result clarifies that the area of the matrix causes this deformation to have a significant impact, highlighting the relevance of this phenomenon in applications where even small deformations can have noticeable effects, such as in composite materials. The analysis of stress concentration within the nanotubes is also an important scope. This helps to understand how the forces applied to the nanotubes are distributed and may be relevant for predicting the behavior of composite materials with nanotubes, their strength, and durability. The result indicates that the electric field depends directly on the area, but in practice, the relationship between the conductor area and the electric field may be more complex. Factors such as the exact geometry of the conductor and edge effects are not fully addressed in the calculation. Although the deformation appears to be significant due to the area of the matrix, the value is extremely small. This could limit the applicability of the model to systems where larger deformations are required or where greater sensitivity is needed.

The model assumes a constant stress concentration in the nanotubes without considering possible variations due to factors such as the orientation of the nanotubes, the distribution of the loads, or possible heterogeneities in the polyethylene matrix. The reality could be more complex, and the actual deformation could vary depending on these factors. The analysis makes ideal assumptions about the behavior of the nanotubes and the matrix, such as uniform polarization and linear response to the applied force. Under real conditions, the nanotubes could experience misalignments, defects, or more complex interactions with the matrix, which would affect the accuracy of the model.

Baughman et al. (2002) demonstrated that carbon nanotubes (particularly single-walled ones) can act as highly efficient actuator materials, capable of generating significant mechanical deformations in response to low-voltage electrical stimuli [24]. Yang et al., 2018, meanwhile, demonstrated that the application of a high-frequency electric field

during the processing of polypropylene nanocomposites with multi-walled carbon nanotubes (MWCNTs) induces effective alignment of the nanotubes within the polymer matrix, which significantly improves their electrical, dielectric, and mechanical properties. This alignment promotes the formation of more efficient conductive networks and increases the stiffness of the material, evidenced by a higher storage modulus. The results confirm that controlling the microstructure using electric fields is an effective strategy for optimizing the functional performance of composite materials, enabling the development of intelligent and multifunctional systems for advanced applications in sensors, actuators, and electroactive devices [27].

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Contribution Role Table

Role	Author(s)
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Data curation	José Aldo Salazar Neri
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Administration Project	Porfirio Roberto Nájera Medina
Resources	Zully Vargas Galarza
Software	José Efraín Ruiz Ramírez
Supervision	Porfirio Roberto Nájera Medina
Validation	José Efraín Ruiz Ramírez
Visualization	José Aldo Salazar Neri
Editorial- Draft	Zully Vargas Galarza
Writing-Revision and editing	Enrique López Chávez



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