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Examining the Impact of Anisotropic Particle Orientation in a Polymer Matrix on the Electrical Properties of Composite Materials

ABSTRACT

A number of works have experimentally shown the significant influence of mechanical stretching on the electrically conductive properties of composite polymer materials. Thus, stretching polymer composite films and filaments can lead to deterioration in electrical conductivity properties which can significantly affect the characteristics of products made from such materials. The research conducted in this study focuses on simulation the impact of anisotropic particle orientation within a polymer matrix and mechanical stretching on the electrical properties of composite materials. Based on the Boltzmann statistics, an expression was obtained that allows predicting the change in electrical conductivity during the stretching of polymer composite samples. The Monte Carlo method was used to simulate the destruction of a percolation chain of conductive particles during stretching.

Keywords: *Polymer composite materials, anisotropic fillers, electrical conductivity, stretching, Monte Carlo simulation*

1. INTRODUCTION

Adding electrically conductive fillers, such as carbon nanoparticles, is a common method used to reduce the resistance of polymer materials [1-15]. These fillers enhance the conductivity of the polymer matrix, allowing for improved electrical performance.

In addition to high conductivity, such composites also exhibit superior mechanical properties compared to metals, are resistant to corrosion. Electrically conductive polymer structures can be used as shielding or antistatic parts of the equipment [7, 14, 16-19]. In modern additive technologies, new polymer composites are used for producing filaments with special properties [20-22]. The relationship between the electrical resistivity of composites and filler concentration exhibits a threshold characteristic [3, 8, 9, 23, 24]. At certain filler concentrations, called critical concentration, filler particles form conducting clusters. These clusters allow electrical current to flow efficiently through the material, reducing the overall resistance of composites compared to the initial resistance of the insulating matrix.

Previous studies [3, 8, 9, 23, 24] have introduced methods for predicting the concentration of fillers in a polymer matrix to identify the threshold concentration required for achieving the desired conductive properties of materials.To describe the percolation process, the researchers used a model of a composite material in the form of a regular cubic lattice [9, 23-25]; the basic algorithm for forming an infinite conducting cluster was the Monte Carlo method. The fillers randomly occupied a position in the cubic lattice, and the geometry of the filler was not taken into account [8, 9, 23, 24]. Next, conditions are applied to identify percolation clusters that can arise as a result of interactions on edges, surfaces or vertices in the three-dimensional case [8, 9]. Samples with high electrical conductivity can even allow the formation of a percolation cluster through one cell [9]. Such modelling is implemented using Monte Carlo simulation; the simulation result well describes the formation of a percolation cluster for isotropic large particles and agglomerates of filler particles. Additionally, the impact of the size of isotropic copper particles on the electrically

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conductive properties of a composite material based on an epoxy binder is also investigated [26]. Several researchers [14, 27-33] have also reported modelling of electrically conductive cluster forming for anisotropic particles like carbon nanofibers and nanotubes. These studies pay attention to the aspect ratio of the fillers. It has been established that a higher aspect ratio significantly increases the likelihood of percolation cluster formation, with simulation results closely aligning with experimental outcomes [30, 31].

However, despite advancements, challenges persist in accurately predicting the electrical conductivity properties in practical, real-world operational scenarios. Experimental works [34-41] have reported the influence of mechanical stretching on the electrically conductive properties of polymer composite materials, where an increase in electrical resistance even by 1 order can lead to a loss of the electrically conductive properties on many orders of magnitude. Thus, in the applications of conductive composites in applications such as protective clothing or covers, where composites experience strong mechanical influence can lead to loss of shielding properties which entail to equipment failure and the negative impact of electromagnetic radiation on humans.

In summary, while modelling the formation of percolation chains has seen significant development, including the study of filler geometry and size, the influence of mechanical deformations on the electrically conductive properties of composite materials remains an open question. There are some experimental results but it is necessary to build the approach for prediction the behaviour of composite conductivity during stretching. This work is dedicated to the examination and modelling of anisotropic filler orientation and its impact on the electrical conductivity and shielding properties of composite materials.

EXPERIMENTAL

The researches [34-39] demonstrated the impact of stretching on the electrically conductive properties of composites with carbon nanofillers. Specifically, when subjected to an elongation value of 5%, the electrical resistance of the fillers increased by 3 times [35-37]. In certain cases, the increase in the electrical resistance was even greater, exceeding an order of magnitude[34, 36, 37]. These experimental results highlight the significant influence of mechanical factors, such as stretching, on the electrical conductive properties of composites.

The influence of orientation stretching on the electrically conductive properties of composite materials is also significant [42, 43]. For the study, in [43] composite filaments based on polypropylene (PP) matrix and carbon nanofibers (CNF) were obtained. The electrical resistivity was measured for two types of samples: without orientation stretching λ=1 and with orientation stretching in 8 times λ=8. The change in orientation stretching is shown on Figure 1 (right) in range of mass fraction. During orientation stretching of polypropylene filament, the polymer molecules are oriented along the stretching axis (Fig. 1, left). Thus, anisotropic particles tend to assume a more energetically favorable state according to the oriented structure of polymer [43].

Based on the experimental results of the composite PP/CNF described above [43], for the experimental study, composite materials based on PP matrix and CNF as a filler were obtained. The mass fraction of CNF was chosen to be 8% due to an electrical resistivity value of less than 120 Ω·cm. Properties of both PP and CNF are provided in Table 1.

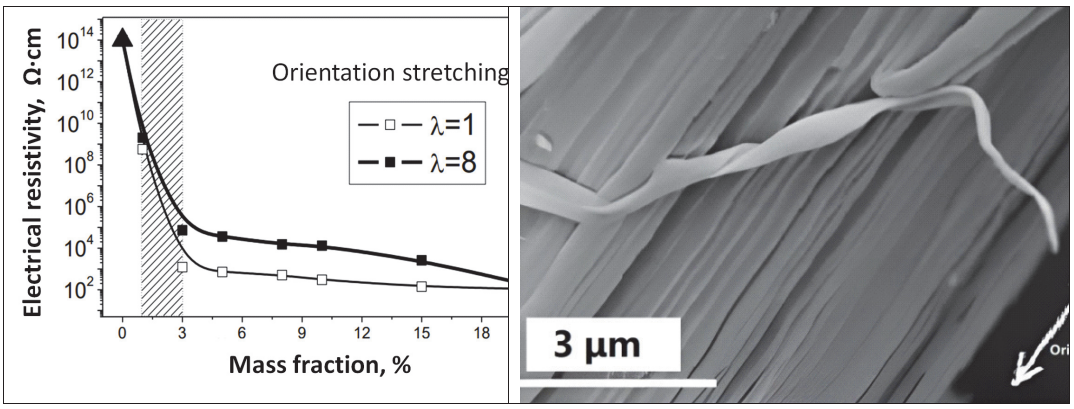

Figure 1. The dependence of electrical resistivity on the filler mass fraction for polymeric filaments in not orientated and orientated conditions (left); the oriented polypropylene filament structure (right) [43].

Table 1. Component characteristics

Material	Characteristics, units of measurement	Value
PP	Melt fluidity index, gr/min	22-30
	Volume electrical resistance of compressed powder, Ω·m	1014
	Poisson ration	0.38
	Melting point, °C	170-176
CNF	Fiber diameter, nm	150
	Fiber length, μm	10-20
	Density, g/cm³	2
	Content of volatile impurities, %	0,1
	Volume electrical resistance of compressed powder, Ω·m	10-4

The samples were obtained using melt technology. CNF as a filler was dispersed in a PP melt within a microcompounder. Mixing was conducted at a temperature of 180 °C for 2 minutes, and then the samples were formed. The samples were obtained in three geometrical forms: blocks, films and filaments. Block-shaped samples were formed by cooling the melt within molds. Film-shaped composites were obtained by rapidly cooling the melt as it exited the slot die. For filament formation, a round die was used. The film and filaments were promptly cooled using compressed air, and then wound onto reels at a constant speed. The films had a width of 25 mm and a thickness ranging from 100 to 200 microns, the filaments had a diameter of 400 μm.

The electrical resistivity of samples with different geometries was measured at room temperature using the four-contact method, and the results are presented in Table 2. At an equal CNF concentration the electrical conductivity of filaments and films is higher than for blocks. This effect can be explained by the difference in the technology of obtaining samples. For the fabrication of the block samples, the composite material was molded in a special form. For films and fibers, a forming dies were installed at the exit of the microcompounder. As it mentioned before, after that films and fibers wound on the reels of the receiving device, λ=1. Thus, the internal structure of composite films and filaments (Fig. 1) have a nominally oriented structure [43].

Table 2. Electrical resistivity of composites with different shape.

Material	Blocks: PP/CNF	Films: PP/CNF	Filaments: PP/CNF
Electrical resistivity	185±12 Ω·m	4.2±0.4 Ω·m	0.20±0.06 Ω·m

This study focuses on investigating the impact of stretching on the electrical conductivity properties of previously obtained samples in form of films and filaments. To conduct the experimental research, a tensile testing machine was upgraded with an electrical circuit to measure current and voltage. The material being studied is subjected to tension. Initially, the mechanical stress (strain) and electrical resistivity values are determined. The films and filaments are then slowly stretched, and the electrical resistivity is measured at control points.

The results show a significant increase in electrical resistivity, with a 1 order of magnitude increase observed at 5% strain (as shown in Figure 2).

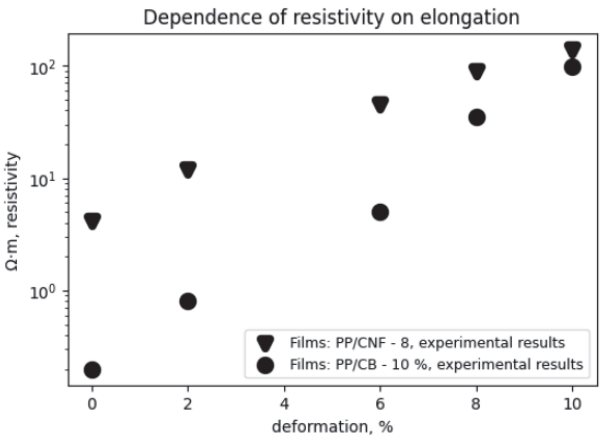

Figure 2. Influence of stretching on the electrically conductive properties of composite materials.

Increase in electrical resistance can be attributed to the reorganizing of the polypropylene structure, specifically the stretching of polymer chains along the direction of mechanical force, resulting in a change in the position of carbon nanofibers. The carbon nanofiber particles tend to align themselves in a more favourable energy state, causing a decrease in the angle relative to the stretching axis and ultimately breaking the percolation chains. The experimental findings suggest that there exists an optimal angle of orientation for the anisotropic filler particles within the matrix, which can lead to the best electrically conductive properties of the composite at a given filler concentration.

RESULTS AND DISCUSSIONS

As a first approximation, we assume that fillers do not agglomerate in order to reveal the dependence of electrical conductivity on the orientation of anisotropic filler particles. A change in filler orientation can occur due to stretching of the composite. In this case, a change in the structure of the polymer matrix molecule occurs, which may entail a change in the orientation of the filler particles and destruction of the percolation cluster, which will entail a deterioration in electrical conductivity properties. To find the optimal angle of orientation, a model using the Monte Carlo method to study the formation of a percolation cluster was developed. The model is implemented in the Python programming language. The primary goal of the model is to examine how the orientation of anisotropic carbon nanoparticles affects the overall structure. However, it is important to note that, for simplicity, the model doesn't take into account the ability of CNF particles to agglomerate in this initial approximation.

The composite material is treated as a two-dimensional square with a side length of "*m*". The anisotropic CNF particles can be represented as linear functions, specifically $y = k \cdot x + b$. The orientation of the fibers will be set relative to the OX axis, where the value of "*k*" will determine the angle of orientation of the anisotropic particles in the composite material. The parameter "*b*" will represent the initial and final coordinates of the segment along the abscissa axis and will be randomly set within the range from 0 to "*m*". The following parameters will be provided as input for the program:

- "*n*": mass fraction of filler in percent
- "*m*": dimension of space (a natural number)
- "α": maximum orientation angle of carbon nanofiber in degrees, ranging from 0° to 90°
- particle aspect ratio.

Firstly, filler particles are randomly generated as segments based on input data. Then, a search is conducted to identify interacting particles, which are determined by the presence of at least one point of intersection between the segments. In the third stage, a percolation cluster is determined using a breadth-first search algorithm. The output of the model is an image that visually represents the distribution of carbon nanofibers in the polymer material. Figure 3 illustrates the distribution model of carbon nanofiber particles with a mass fraction of 8% in a polymer matrix, considering an orientation angle of anisotropic particles up to 40°. The influence of the orientation of carbon nanofibers on the electrical conductive properties of the composite material is examined at a filler concentration of 8%. The simulation is conducted for the maximum orientation angle of carbon nanofibers (α) ranging from 0° to 90° with a step of 5°. Figure 4 presents the results of modeling the formation of a percolation cluster or long chains for five different types of angles.

The probability of the percolation cluster formation is calculated as the proportion of successful formation attempts for all simulations. The program performs the simulation 100 times, in each case the algorithm searches for a percolation chain. If a percolation chain has been formed, then the algorithm considers the attempt successful. All successful attempts are summed up.

Figure 3. Distribution of carbon nanofibers in the polymer matrix (the filler concentration is 8%): red – the percolation cluster, yellow - long chains of interacting particles in the absence of a percolation cluster, gray - interacting particles not included in long chains, black - non-interacting particles.

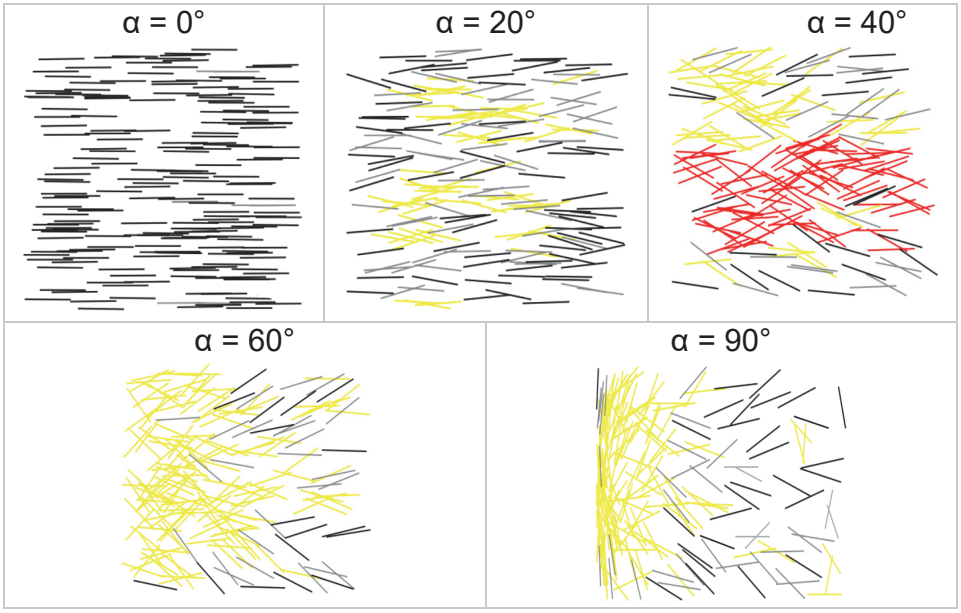

Figure 4. Results of modelling the orientation of carbon nanofibers in a composite material at a filler concentration of 8%.

In the absence of orientation along the abscissa axis (in this case, we take the maximum orientation angle α = 90°), the percolation cluster is not formed.A similar result is confirmed experimentally for samples in the form of blocks, the formation of which is carried out by rapid cooling of the solidification of the melt in the mold. The probability of formation of a percolation chain is zero. During the formation of block samples, the particles of carbon nanofibers are randomly distributed in the volume, and the electrical resistivity is 2 orders of magnitude higher than for film samples, in which orientation is present due to the method of obtaining samples. As the maximum angle decreases to 60°, the probability of the formation of a percolation cluster greatly increases and reaches 70%.

The maximum probability of formation of a percolation cluster 97-100% is achieved at the maximum value of the orientation angle in the range from 35° to 55°. This practically corresponds to the formation of unoriented film materials. With a further decrease in the maximum orientation angle of nanofibers in the material, the probability of the formation of a percolation cluster decreases, and at a value of α = 0°, it is unlikely that one segment will intersect two. Such a deterioration in the electrically conductive properties is described by the orientational stretching of film composite materials.

Thus, we can conclude that the highest probability of the formation of a percolation cluster in a composite material based on a polymer matrix and carbon fillers can be achieved by orienting carbon nanofibers along some axis. Anisotropic carbon nanoparticles are considered as dipoles, thus, carbon nanofiber particles have some orientation relative to the film drawing axis, which is confirmed by micrographs of samples [26, 41].

As the strain increases, the orientation angle of the anisotropic particles decreases. Thus, in structures which there is no orientation (the maximum angle between the axis of the orientation stretching and the axis of the anisotropic particle is 90°), the orientation angle decreases upon stretching, and the probability of the formation of a percolation cluster increases until a certain value is reached. The simulation results make it possible to predict that the maximum angle between the axis of the orientation stretch and the axis of the anisotropic particle is in the range of 35-55°. Thus, orientation upon stretching can improve the properties of composite materials. So, at equal concentrations, block and film materials have different values of electrical resistance block materials have a greater value. This is an agreement with the Monte Carlo simulation however it is worth noting the limits of reliability of modelling. A similar scenario takes place only at filler concentrations close to the threshold value.

In oriented structures, there is a loss of electrically conductive properties, which is confirmed experimentally. In this case, the orientation angle continues

to decrease and, at a certain value, the conductive chains are destroyed. Modelling suggests that at a maximum angle between the axis of the orientation stretching and the axis of the anisotropic particle of 35° or less, the probability of destruction of the percolation cluster increases.

In this section, a model is constructed that allows one to predict the value of the electrical resistance of a composite material depending on stretching. Electrons are considered as carriers of electric charge in composite materials. It is assumed that electrons are a classical non-degenerate gas, taking into account the amorphous structure of the matrix and the random distribution of the filler. If the electron gas is in thermodynamic equilibrium, such a system obeys Boltzmann-Maxwell statistics. The charge transfer from one conducting particle to another is carried out due to the electron-phonon interaction. Under mechanical action on the sample and a change in the orientation of the filler in the matrix, a change in the internal energy occurs, which in turn leads to an increase in the thermal vibrations of the lattice. An electron under the action of thermal vibrations of the lattice performs a transition from state 1 to state 2, overcoming some energy barrier, height H and width δ. The width and height of the barrier are linearly related to the mechanical effects on the system.

In accordance with Boltzmann-Maxwell statistics, we write the probability of overcoming the energy barrier from state 1 to state 2 in the case of a material transition from a non-conductive to a conductive state

$$W_{12} = \omega_{12} e^{\frac{-H-eE}{k_b T}}, \quad (1)$$

where *e* is the electron charge, *E* is the field strength, k_b is the Boltzmann constant, *T* is the temperature, ω_{12} is the fraction of particles that have passed from state 1 to state 2. He barrier value H is a function inversely proportional to two variables: filler concentration ϑ and deformation ε (orientation angle α):

$$H = H(\vartheta, \varepsilon(\alpha))$$

Such a process will be considered reversible, i.e. a transition from state 2 to state 1 is possible, with probability

$$W_{21} = -\omega_{21} e^{\frac{H-eE}{k_b T}}, \quad (2)$$

where ω_{21} is the fraction of particles that have passed from state 2 to state 1. The difference in expressions (1) and (2) gives us the dependence of the resistivity change on the height of the potential barrier, i.e. on deformation, concentration of fillers, and orientation angle of anisotropic particles:

$$\delta\rho = \rho_0 \varepsilon cosh(\gamma \mathrm{H}) \quad (3)$$

- electrical resistance in the absence of mechanical influences. T

As objects of study, in addition to the experimental results shown in Figure 1, we will consider the experimental dependencies presented in works [35, 36]. In [35], PEO (polyethylene oxides) was used as a polymer matrix, carbon nanotubes were used as fillers, the filler concentration was 3%. In [36], materials based on rubber filled with carbon black were experimentally studied. We believe that conductivity is related to the deformation and mechanical properties of the matrix, thus taking into account the Poisson's ratio.

$$\rho = \rho_0 (1 + \varepsilon \cdot cosh(\varepsilon \cdot \gamma)) \quad (4)$$

Figure 5 shows good agreement between the obtained mathematical expression and the experimental results, thus the expression for resistance can be used to predict the properties of polymer composite materials.

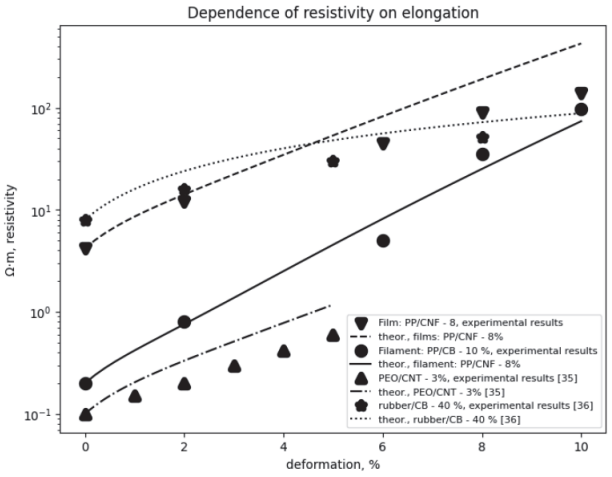

Figure 5. Theoretical and experimental dependences of stretching deformation on the electrically conductive properties of composite materials

CONCLUSIONS

This study investigates how mechanical stretching and the resulting alignment of anisotropic particles within composite materials affect their electrical conductivity. Our findings reveal that orienting fillers, such as carbon nanofibers, between 35° to 55° relative to

a specific axis significantly enhances the likelihood of percolation cluster formation. Our simulations closely align with experimental results. By strategically orienting these particles without altering filler concentration, we can markedly enhance electrical conductivity, achieving the necessary electrical resistivity for shielding properties in composite polymer materials and their derived products. Notably, materials exposed to high mechanical stress risk losing their electrical conductivity and subsequent shielding properties, posing safety hazards in composite material-based products. One viable solution to counteract the decline in electrical conductivity during operation is by increasing filler concentration. Moreover, our work derives an expression rooted in Boltzmann statistics, offering insight into predicting the rise in electrical resistance when film samples undergo stretching. This expression holds promise in forecasting the performance of composite polymers, particularly in film and textile formats utilized for shielding against electric fields.

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IZVOD

ISPITIVANJE UTICAJA ANISOTROPNE ORIJENTACIJE ČESTICA U POLIMERNOJ MATRICI NA ELEKTRIČNA SVOJSTVA KOMPOZITNIH MATERIJALA

Veliki broj radova je eksperimentalno pokazao značajan uticaj mehaničkog istezanja na elektroprovodna svojstva kompozitnih polimernih materijala. Dakle, istezanje polimernih kompozitnih filmova i filamenata može dovesti do pogoršanja svojstava električne provodljivosti što može značajno uticati na karakteristike proizvoda napravljenih od takvih materijala. Istraživanje sprovedeno u ovoj studiji se fokusira na simulaciju uticaja anizotropne orijentacije čestica unutar polimerne matrice i mehaničkog istezanja na električna svojstva kompozitnih materijala. Na osnovu Bolcmanove statistike dobijen je izraz koji omogućava predviđanje promene električne provodljivosti tokom istezanja uzoraka polimernih kompozita. Monte Karlo metoda je korišćena za simulaciju uništavanja perkolacionog lanca provodnih čestica tokom istezanja.

Ključne reči. *Polimerni kompozitni materijali, anizotropna punila, električna provodljivost, istezanje, Monte Karlo simulacija*

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