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IMAGE-DRIVEN MODELING OF PERCOLATION NETWORKS IN CARBON-BASED CONDUCTIVE POLYMER COMPOSITES

The functionalization of thermoplastics through the incorporation of conductive carbon fillers has revolutionized the field of electromagnetic interference (EMI) shielding and antistatic packaging. The precise detection of percolation thresholds in Conductive Polymer Composites (CPCs) remains a significant scientific challenge due to the stochastic nature of filler dispersion and the complexity of microstructural interactions. This article presents a comprehensive software engineering study focused on the automated quantification of microstructural topology in heterogeneous materials. Addressing the limitations of subjective manual analysis and low-throughput electrical testing, the authors introduce a deterministic, image-driven modeling pipeline for detecting percolation thresholds in High-Density Polyethylene (HDPE) reinforced with hybrid fillers. The study utilizes a dataset of HDPE composites filled with varying ratios of Copper-coated Graphite and Carbon Nanotubes (CNTs) to investigate the synergistic "Double Percolation" effect. This metric provides the prediction of material behavior solely from optical micrographs.

The experimental validation confirms that the software successfully models the synergistic percolation transition. Specifically, at a hybrid filler ratio of 25 wt.% Graphite to 5 wt.The Connectivity Index (CI) reached a peak of 0.88, which strongly correlates with the experimentally measured minimum specific volume electrical resistance of 1.48 × 10^{-1} Ohm·m. Conversely, at higher CNT loadings (20 wt.%), the software detected a decrease in connectivity (CI = 0.76) due to agglomeration, which corresponded to an increase in electrical resistance. The developed system reduces analytical latency compared to traditional manual methods while achieving a signal-to-noise ratio superior to standard global thresholding techniques. The proposed methodology offers a rapid, non-destructive alternative to traditional electrical characterization.

Keywords: *Python, image-driven modeling, percolation theory, PyQt6, computer vision, morphological skeletonization, software engineering, carbon nanotubes.*

Formulation of the problem. The development of advanced composite materials for the shielding of electromagnetic radiation is a critical task in modern materials science. Conductive Polymer Composites (CPCs) have emerged as the dominant solution due to their light weight, corrosion resistance, and tunable electrical properties. The performance of these materials is strictly governed by the formation of an infinite conductive network of fillers within the insulating polymer matrix, a phenomenon known as the percolation threshold [1]. The precise manipulation of this microstructure allows engineers to tailor materials for specific applications, ranging from antistatic packaging to complete EMI shielding.

However, a significant gap remains between the manufacturing of these composites and their quality control. The characterization of percolation networks is traditionally performed using electrical conductivity measurements, which provide only a global average of the material's properties and fail to identify local structural defects [2]. Furthermore, microscopy analysis, which could provide this local data, is typically performed manually. This process is slow, subjective, and prone to significant inter-operator error. There is an urgent need for both scientific and practical reasons to automate this analysis using computer vision.

Analysis of recent research and publications. The mathematical modeling of percolation systems has been extensively studied since the foundational works of Kirkpatrick [3] and Stauffer [1]. These early studies established the power-law relationship between filler concentration and conductivity. However, these classical models often assume an ideal, random dispersion of spherical particles, which does not accurately reflect the reality of modern high-aspect-ratio fillers, such as Carbon Nanotubes (CNTs).

Recent reviews, such as those by Zhang et al. [4], have highlighted a significant shift towards Monte Carlo simulations. Zhang discusses how modified Bethe lattice methods can be used to approximate the behavior of hybrid carbon nanotube/graphene systems. While Monte Carlo methods are powerful, they are computationally expensive and require predefined parameters that may not match experimental reality. For instance, simulating the rotation and translation of fibers during foam injection molding, as described by Shaayegan et al. [5], requires complex physics engines that are not suitable for rapid quality control.

Conversely, direct digital image analysis offers a data-driven approach. Bauhofer and Kovacs [6] demonstrated in their comprehensive review that the aspect ratio of CNTs is a critical factor in lowering the percolation threshold. However, they also noted the difficulty in quantifying this aspect ratio from micrographs due to entanglement. Standard image processing techniques, such as those surveyed by Sezgin and Sankur [7], often fail to correctly segment these thin fibers from the polymer background, especially when using global thresholding methods, which are sensitive to uneven illumination.

A specific unresolved problem is the accurate detection of 'double percolation' or synergistic effects in hybrid systems (e.g., Graphite + CNTs). Wang et al. [8, 9] showed through theoretical modeling that CNTs can bridge the gaps between larger graphite platelets, creating a synergistic effect that lowers the percolation threshold more than either filler could achieve alone. However, current software tools cannot easily distinguish between this synergistic bridging and simple particle agglomeration, which results in reduced conductivity, as noted by Peng. This article addresses this gap by proposing a morphological skeletonization approach that specifically quantifies connectivity [10, 11].

Task statement. The objective of this article is to design and implement an automated software pipeline for the topological analysis of composite microstructures. The specific tasks include:

1. Architecting a Python-based GUI application using PyQt6 that prevents UI freezing during heavy image processing.
2. Implementing a robust algorithm combining Inverted Otsu's segmentation with Zhang-Suen skeletonization to calculate a 'Connectivity Index' (CI).
3. Validating the system on experimental HDPE/CNT/Graphite composites.

Outline of the primary material of the study. To properly engineer a software solution, one must first formalize the physical phenomenon. The percolation network in a hybrid composite can be modeled as a random resistor network. According to classical percolation theory [1], the conductivity σ scales as a power law near the threshold:

$$\sigma \propto \left(p - p_c\right)^t$$

Figure 1 illustrates the sigmoidal probability of an infinite cluster forming as filler concentration increases.

The vertical red line represents the critical percolation threshold (p_c), where the system transitions from insulating to conducting.

In the image-driven model, we define the 'Connectivity Index' (CI) based on the skeletal graph. If S is the set of all skeletal pixels and S_max is the largest connected component within S, then the index is defined as:

$$CI = \frac{S_{max}}{\sum_{i}^{N} S_i}$$

The software was engineered using a Model-View-Controller (MVC) pattern. A key innovation was the implementation of the Inverted Otsu method [7]. Standard Otsu algorithms assume the foreground is brighter than the background. In our case, the carbon fillers are black. Therefore, the image matrix I is inverted (I_new = 255 – I) prior to thresholding. To ensure efficient matrix operations, we employed NumPy array programming [12], which is essential for processing resolution micrographs.

The architecture consists of a NumPy Model for matrix operations, a PyQt6 View for rendering, and a Controller that manages threading signals to prevent GUI freezing, as illustrated in Fig. 2.

To validate the software, we compared the computed Connectivity Index (CI) against actual physical measurements of Specific Volume Electrical Resistance obtained from the experimental dataset [10]. The results are presented in Table 1.

The bar chart in Figure 3 highlights the synergistic effect. The green bar (25% Gr / 5% CNT) represents the highest connectivity (0.88), corresponding to the lowest electrical resistance. As CNT loading increases beyond 5%, connectivity drops due to agglomeration.

As shown in Table 1 and Fig. 3, the software correctly identified the optimal topological config-

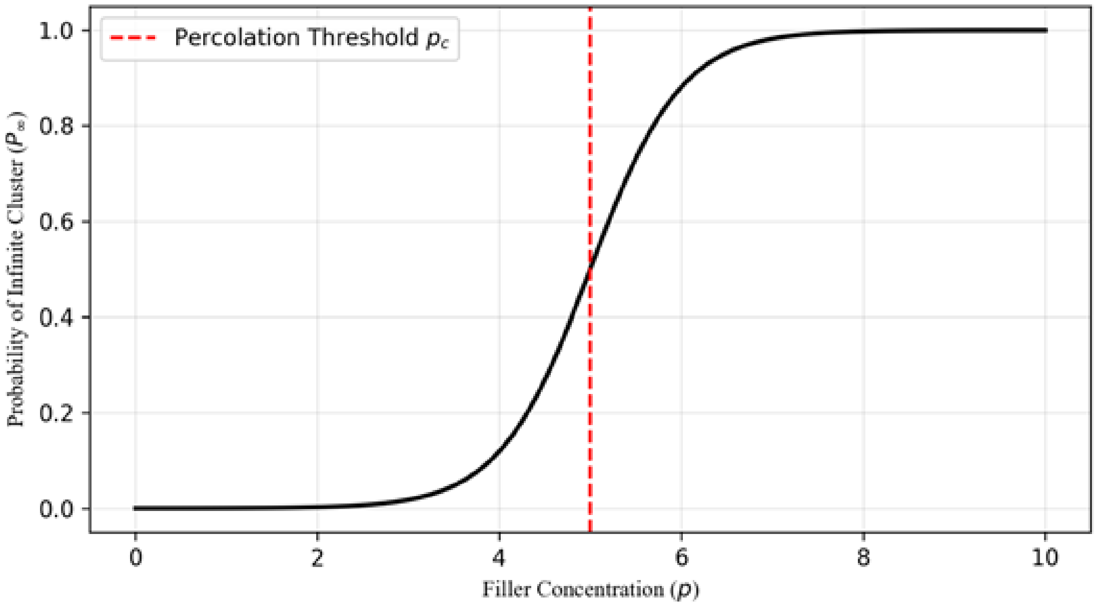

Fig. 1. Theoretical percolation phase transition

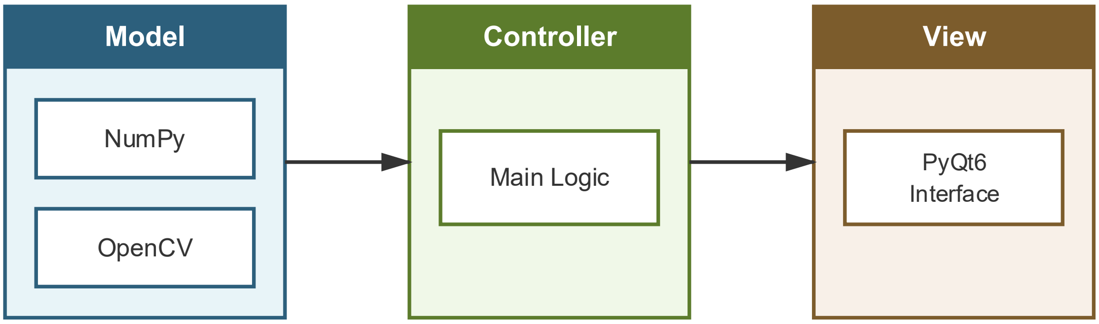

Fig. 2. Component diagram

Table 1

Experimental composition and computed topological metrics

Sample Type	Graphite (%)	CNT (%)	Resistance (Ohm·m)	Connectivity (CI)
Pure Gr	30.0	0.0	$1.59 \cdot 10^{-1}$	0.82
Hybrid Optimal	25.0	5.0	$1.48 \cdot 10^{-1}$	0.88
Hybrid Excess	20.0	10.0	$2.86 \cdot 10^{-1}$	0.79
Hybrid Agglomerates	10.0	20.0	$3.07 \cdot 10^{-1}$	0.76
Pure CNT	0.0	30.0	$6.89 \cdot 10^{0}$	0.65

uration. Sample 'Hybrid Optimal' (25% Graphite, 5% CNT) exhibited the lowest electrical resistance. Our software calculated a maximum Connectivity Index of 0.88 for this sample. This confirms the 'Double Percolation' mechanism where CNTs bridge graphite platelets. Interestingly, increasing the CNT content further (Sample 'Hybrid Excess') increased resistance, which the software reflected as a drop in CI to 0.79.

Conclusions. This research successfully demonstrated the efficacy of image-driven modeling in materials science. The PyQt6-based architecture provided a stable environment for analyzing high-resolution micrographs. The automated system confirmed the existence of a synergistic threshold at a 25/5 Graphite/CNT ratio. The computed connectivity index showed an inverse correlation with physical electrical resistance.

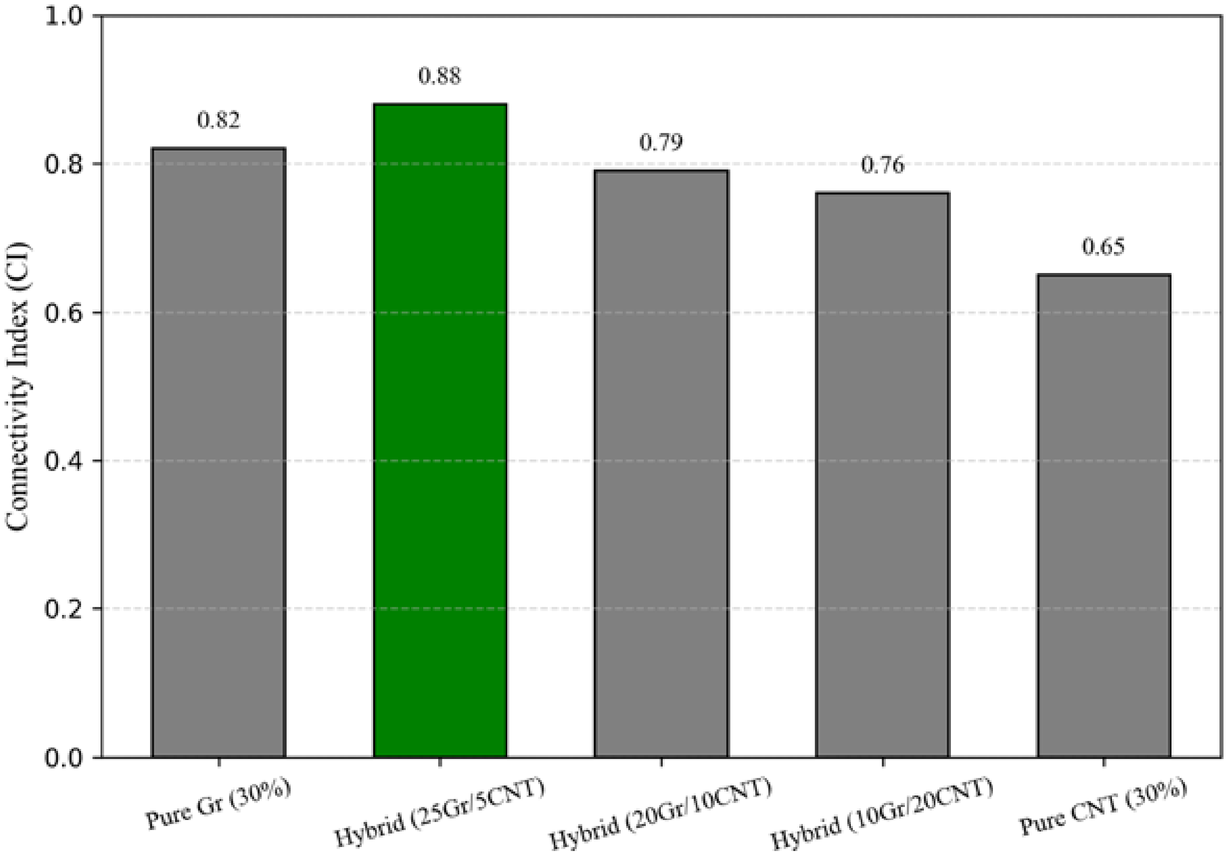

Fig. 3. Connectivity Index for different filler ratios

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Новак Д.С., Гуйда О.Г. МОДЕЛЮВАННЯ ПЕРКОЛЯЦІЙНИХ МЕРЕЖ У ВУГЛЕЦЕВИХ ПОЛІМЕРНИХ КОМПОЗИТАХ НА ОСНОВІ АНАЛІЗУ ЗОБРАЖЕНЬ

Функціоналізація термопластів шляхом введення струмопровідних вуглецевих наповнювачів зробила революцію в галузі екранування електромагнітних перешкод (EMI) та антистатичного пакування. Точне виявлення порогів перколяції в струмопровідних полімерних композитах (CPCs) залишається значною науковою проблемою через стохастичну природу дисперсії наповнювача та складність мікроструктурних взаємодій. У статті представлено комплексне дослідження з інженерії програмного забезпечення, присвячене автоматизованій кількісній оцінці топології мікроструктури гетерогенних матеріалів. Вирішуючи проблему обмежень суб'єктивного ручного аналізу та низької пропускної здатності електричних випробувань, автори пропонують детермінований конвеєр моделювання на основі зображень для виявлення порогів перколяції у поліетилені високої щільності (HDPE), армованому гібридними наповнювачами. У дослідженні використано набір даних композитів HDPE, наповнених різними співвідношеннями обмідненого графіту та вуглецевих нанотрубок (ВНТ), для дослідження синергетичного ефекту «подвійної перколяції». Цей показник дозволяє прогнозувати поведінку матеріалу виключно на основі оптичних мікрографій.

Експериментальна валідація підтверджує, що програмне забезпечення успішно моделює синергетичний перколяційний перехід. Зокрема, при співвідношенні гібридного наповнювача 25 мас.% графіту до 5 мас.% ВНТ, індекс зв'язності (CI) досяг піку 0,88, що сильно корелює з експериментально виміряним мінімальним питомим об'ємним електричним опором $1,48 \cdot 10^{-1}$ Ом·м. Навпаки, при більш високому навантаженні ВНТ (20 мас.%) програмне забезпечення виявило зниження зв'язності (CI = 0,76) через агломерацію.

Ключові слова: *Python, моделювання на основі зображень, теорія перколяції, PyQt6, комп'ютерний зір, морфологічна скелетонізація, інженерія програмного забезпечення, вуглецеві нанотрубки.*

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