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Implement Explainable Machine Learning to Improve Conductivity in Polymer-CNT Nanocomposites: Supporting Adaptive, Flexible, and Long-Lasting IoT Wrap-Around Electronics Applications

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Abstract

The rapid growth of Internet of Things (IoT) technologies requires electronic components that are adaptable, lightweight, and durable, and that can continue to function well in diverse contexts and circumstances. Polymer–carbon nanotube (CNT) nanocomposites have become interesting choices for these kinds of uses because they are more flexible, conduct electricity better, and can be made to fit specific needs. However, improving conductivity in these heterogeneous systems remains a major challenge because of the complex relationships between polymer form, CNT dispersion, interfacial interactions, and processing conditions. This study introduces an explainable machine learning (XML) framework designed to systematically model and enhance conductivity in polymer-CNT nanocomposites, ensuring transparency and interpretability in predictions. The methodology integrates feature attribution techniques with interpretable model architectures to elucidate critical attributes, such as CNT concentration, aspect ratio, polymer crystallinity, and filler alignment, that significantly influence charge transport pathways. The architecture makes it possible to use adaptive tuning strategies to attain the optimum conductivity without giving up flexibility, durability, or ease of fabrication. To test the results, conductivity tests are taken on different compositions and processing methods. To help with material development, model predictions are employed. The knowledge gained helps to make polymer-CNT nanocomposite systems that are flexible, energy-efficient, and long-lasting for wrap-around IoT electronics, which need to be able to bend, stretch, and change with the environment all the time. Adding explainability not only makes things work better, but it also fosters trust, speeds up the search for new materials, and gives a plan for using this method on more multifunctional nanocomposites. The approach ultimately advances next-generation, sustainable electronic materials by combining data-driven optimization with basic physical laws.

Keywords: Electrical Conductivity Optimization, Flexible Electronics, Adaptive Optimization Framework, Material Design Interpretability, Long-Term Durability, Polymer–Carbon Nanotube Nanocomposites, IoT Wrap-Around Devices.

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INTRODUCTION

The Internet of Things (IoT) has grown quickly, and this has impacted how individuals in modern cultures use technology. In ordinary life, it has made it feasible for sensors, gadgets, and smart systems to work together without any complications [1,2]. For the Internet of Things (IoT) to work, it needs materials that can change to fit diverse situations while yet being mechanically flexible, electrically stable, and long-lasting. These materials are employed in things like smart packaging, wearable communication systems, healthcare monitoring patches, and automation in factories. Silicon-based electronics that are inflexible and old-fashioned are not ideal for these kinds of uses since they can't bend, stretch, or fold without breaking [3]. Because of this limit, people are more interested in alternate materials that can support flexible, wrap-around IoT devices that can take constant bending and stress from the environment. Polymer-based composites enhanced with carbon nanotubes (CNTs) are a fascinating material due to its lightweight nature, customizable electrical properties, and inherent flexibility [4,5]. However, attaining reproducible and optimal conductivity in polymer-CNT systems continues to pose a considerable challenge, due to their intricate hierarchical microstructure and the fragile equilibrium of nanoscale interactions.

Polymer-CNT nanocomposites show electrical conductivity mainly through the formation of percolation networks, where evenly spaced CNTs make conductive channels that run through the polymer matrix without interruption [6]. But conductivity is greatly affected by a number of factors that are linked to each other, such as the concentration of fillers, the aspect ratio of CNTs, the crystallinity of the polymer, the adhesion between layers, and the processing conditions. The electrical routes won't be even if the CNTs don't spread out well or stick together. If there is too much filler, the material might not be as flexible or easy to work with [7]. Moreover, the enduring stability of conductivity in relation to environmental fluctuations, such as humidity, temperature shifts, and cyclic mechanical stress, is still not well understood. There is a problem that needs to be tackled in various ways because of the trade-offs between making things more conductive, more durable, and easier to build. Standard trial-and-error experimental methods are costly and time-consuming, and conventional computer models sometimes lack the accuracy to represent nonlinear dependencies in such systems [8]. We need sophisticated, data-driven ways to figure out these intricate links so that we can change the conductivity of polymer-CNT in a systematic way for IoT applications that need to be adaptable.

In the last few years, machine learning (ML) has become a game-changing method in materials science. By learning from data and developing very accurate predictions about what will happen, it helps speed up discovery and optimization. Some of the machine learning (ML) methods that have been used to guess the mechanical strength, thermal conductivity, and electrochemical performance of a wide range of new materials are regression models, decision trees, and neural networks [9–11]. For polymer nanocomposites, ML may use both experimental and simulation data to simulate nonlinear relationships between structural, compositional, and processing parameters. This helps researchers find the best configurations [12]. But traditional ML models frequently work like black boxes, making correct predictions without showing how they work. This can speed up performance optimization, but it makes it harder for researchers and engineers to understand results, check scientific ideas, or share knowledge between different material systems. These kinds of limits are very important in high-stakes situations like flexible IoT electronics, where reliability, sustainability, and flexibility are all very important [13,14].

To overcome the shortcomings of opaque black-box models, explainable machine learning (XML) frameworks have become popular, providing both predicted accuracy and interpretability [15]. Researchers can use XML methods like SHAP (SHapley Additive exPlanations), LIME (Local Interpretable Model-agnostic Explanations), and interpretable deep learning architectures to figure out how important different input features are, find the main factors that affect material performance, and get causal insights into how structure and property are related. Researchers can use XML to find out what factors affect conductivity in polymer-CNT nanocomposites, such as the state of CNT dispersion, the alignment of fillers, or the interactions between the matrix and fillers. They can also learn how secondary properties change under different situations [16,17]. XML is important because it makes adaptive tuning strategies possible. This means that conductivity may be improved without sacrificing flexibility or durability, which directly meets the needs of IoT wrap-around devices. Also, XML's openness helps materials scientists, engineers, and industry stakeholders trust and embrace it, which closes the gap between computer prediction and physical interpretation.

Combining explainable ML with polymer-CNT nanocomposites could greatly improve the future generation of adaptive IoT circuits. Wrap-around devices, including conformal health monitors, smart textiles, wearable antennas, and flexible environmental sensors, need materials that not only have good electrical conductivity but also keep working well when they are bent and stressed by the environment [18]. Wearable biosensors need to keep sending signals reliably even when they are stretched over and over again. Smart packaging's flexible antennas need to be able to handle changes in humidity and temperature without losing their ability to conduct electricity. XML-driven conductivity optimization exposes trade-offs and lets designers pick materials that work for both purposes [19]. This makes it easy to meet both of these needs. XML may also help make products that are both eco-friendly and long-lasting faster, which means less need to overengineer materials and cheaper costs over time. This goes along with the global goal of producing technologies that are better for the environment and consume less energy. IoT ecosystems will need a lot of these technologies.

This research focuses on utilizing explainable machine learning to improve conductivity in polymer-CNT nanocomposites, with the objective of delivering adaptable, flexible, and durable IoT wrap-around electronics. The study develops an XML framework that integrates experimental data, feature attribution methods, and interpretable predictive models to clarify the complex connections among structural, compositional, and processing parameters [20]. The framework not only effectively predicts conductivity, but it also provides valuable insights into the primary factors influencing charge mobility inside materials. Experimental validation confirms the robustness of the technique, demonstrating improved conductivity optimization across diverse composite formulations and processing routes. This study signifies a dual enhancement by amalgamating predictive capability with interpretability: (i) it enables systematic, adaptive optimization of polymer-CNT conductivity tailored for IoT applications, and (ii) it presents a transferable methodology applicable to other multifunctional nanocomposites. This work establishes XML as a crucial enabler for the integration of data-driven optimization with physical understanding, hence advancing the creation of sustainable, high-performance materials for the Internet of Things age. The rest of this paper is organized like this: Section 2 examines pertinent literature, whereas Section 3 elaborates on the proposed methodology. Section 4 reveals what happened in the experiments, and Section 5 talks about the most essential ones. Lastly, Section 6 wraps up the study and talks about where future research should go.

LITERATURE REVIEW

Percolation processes, tunneling transport, and interfacial physics are the main things that affect how polymer–carbon nanotube (CNT) nanocomposites behave electrically. Early research shown that a specific critical volume fraction of carbon nanotubes (CNTs) creates a conductive network within an insulating polymer matrix, and that the percolation threshold can be reduced by utilizing high aspect ratio fillers and enhancing dispersion [21,22]. Later research improved on these ideas by simulating how electrons move as a mix of direct contacts and tunneling through nanoscale polymer gaps, where the distance between tubes, their alignment, and the resistance of the junctions control how well electricity flows. In addition to composition, microstructural descriptors—network connectedness, tortuosity, clustering coefficient, and path redundancy—have been identified as quantitative predictors of macroscopic conductance [23]. Imaging-guided reconstructions (SEM/TEM/μCT), representative volume element (RVE) simulations, and finite element/tunneling resistance networks have been employed to connect different scales, demonstrating that little alterations in dispersion state or alignment can result in significant variations in conductivity. However, standard analytical models (effective medium theory, classical percolation scaling) frequently inadequately represent the multivariate, nonlinear interactions between filler geometry, polymer morphology, and processing history, necessitating additional data-driven methodologies.

Consequently, processing-structure-property linkages have emerged as a fundamental theme. Solution casting and melt compounding provide different states of dispersion and interfacial tension; shear-assisted processes like extrusion, 3D printing, and blade coating affect alignment; and post-processing methods like annealing, stretching, and solvent vapor exposure can make conductive pathways rougher or smoother [24]. Chemical functionalization and compatibilizers enhance interfacial adhesion and stabilize dispersion; however, they may interfere with π-conjugation and elevate junction resistance, resulting in a compromise between mechanical integrity and electrical performance. Materials that last despite bending, stretching, and being exposed to the elements (humidity, temperature variations, sweat/saline for wearables) have been made using elastomeric matrices, wavy/serpentine structures, and self-healing chemistries that restore percolation after microcracking [25]. The literature, however, demonstrates that there is a lot of diversity between labs. This is probably because the precursors, the procedures for dispersion, and the methodologies employed for metrology are all different. This variation underscores the imperative for standardized datasets and robust statistical design principles, especially for devices intended for extensive, long-term IoT implementation, where drift, hysteresis, and fatigue of the conductive network constitute critical failure modes.

The concurrent progress in flexible and wearable electronics has highlighted application-driven standards that meticulously assess polymer–CNT systems. For conformal sensors, stretchy interconnects, and flexible antennas, conductivity must coexist with low modulus, good fatigue resistance, and stable impedance with frequency and strain [26,27]. Studies on piezoresistive and bio-interfacing devices demonstrate that gauge factor, strain range, and recovery kinetics are markedly affected by microstructural reserve connectivity, which denotes the redundancy of parallel pathways that allows networks to maintain conductance during strain-induced openings at specific junctions. For RF and antenna applications, homogeneity of sheet resistance, skin depth, and stability of humidity and temperature become very important. Multilayer structures (conductive layer + barrier + encapsulant) are said to last longer, but they also make processing harder and increase the chance of delamination. The key problem in these circumstances is still multi-objective optimization: how to improve conductivity without losing flexibility, adhesion, manufacturability, or eco-toxicity. Traditional design-of-experiments is useful, but the combinatorial space of CNT type, loading, dispersion chemistry, rheology, shear history, and curing profile quickly becomes too big to handle. This is where machine learning has started to aid [28].

People have been using machine learning (ML) more and more on polymer nanocomposites to anticipate properties, develop things in reverse, and improve processes. Random forests, gradient boosting, Gaussian processes, and neural networks have forecasted conductivity, percolation thresholds, and mechanical performance based on parameters including composition, CNT geometry, rheological indicators, and image-derived microstructure statistics [29]. Active learning and Bayesian optimization have lowered the costs of experiments by directing measurements to useful areas, while transfer learning has used knowledge from one polymer matrix or CNT family to another [30]. Graph-based and physics-informed machine learning (PIML) models have included restrictions from percolation theory and tunneling transport, resulting in enhanced extrapolation and logically constrained predictions. However, two gaps remain: (i) data scarcity and heterogeneity (mixed protocols, inconsistent feature definitions, small-N datasets) that hinder generalization; and (ii) the "black box" problem [15], high predictive accuracy coupled with limited mechanistic insight, complicating trust, regulatory acceptance, and portability across applications (e.g., transitioning from strain-sensing films to wrap-around antennas).

Explainable machine learning (XML) fills in these gaps by putting interpretability on the same level as accuracy. Feature permutation importance, partial dependency and accumulated local effects (ALE), SHAP, and LIME are model-agnostic techniques that measure contributions and interactions. They show which factors have the biggest effect on conductivity and under what conditions [31]. Global surrogates, like sparse symbolic regressors and distilled tree ensembles, describe rules at the system level. Local explanations, on the other hand, show the causes of composition- or process-specific events, as when aspect ratio is more important than interfacial chemistry for tunneling. Recent research combines XML with uncertainty quantification to identify incorrect predictions and with counterfactual analysis to propose minimum adjustments (e.g., a slight enhancement in CNT alignment or a modest reduction in solvent-exchange time) to achieve objectives. Integrating XML with microstructure-aware features—such as network connectivity metrics, alignment order parameters, and inter-junction spacing distributions derived from images—has initiated a connection between "what the model learned" and "what the microstructure is," providing a mechanistic link that was lacking in previous black-box workflows. Nonetheless, consistent pipelines for image processing, feature extraction, and explanation reporting are still not well-developed, and not many studies rigorously test how stable explanations are when datasets change or various processing paths are used.

METHODS

In order to use polymer-carbon nanotube (CNT) nanocomposites in adaptive, flexible, and long-lasting IoT wrap-around electronics, both materials engineering and data-driven design need to make progress. Traditional strategies for improving conductivity in polymer-CNT systems are frequently limited by the complicated interactions between CNT dispersion, alignment, percolation thresholds, and the polymer matrix's interfacial interactions. This complexity makes it very hard to get stable conductivity whether there is mechanical stress, bending, or changes in the environment. The suggested design uses explainable machine learning (XML) to get over these problems by looking at big datasets from experimental synthesis, computational simulations, and real-time feedback from IoT devices (see Figure 1). XML helps researchers find the most important factors that affect conductivity, like CNT volume fraction, polymer crystallinity, and curing conditions. These factors may then be systematically adjusted to improve performance. The first step in creating an architectural model is to get data. This means getting datasets from several places, like measurements of electrical conductivity, pictures of microstructures, and how stress and strain change when the environment changes. These datasets are put into modules for pre-processing and feature engineering, where significant microstructural [23] descriptors are extracted out and parameters are standardized. The explainable machine learning layer then employs models like SHAP (Shapley Additive Explanations) or LIME (Local Interpretable Model-Agnostic Explanations) [15,31] to figure out what predictions made by advanced learners like graph neural networks or ensemble tree models mean. The explainability layer does more than just look for connections; it also demonstrates how conductivity channels work. For example, it can highlight how specific CNT alignments under stress make electron tunneling better or how the flexibility of polymers helps keep percolation networks operating as they bend and straighten out. Finally, the feedback and optimization module uses XML data and hybrid computational-experimental loops to assist come up with design ideas that can change [30]. Then, these rules are utilized to adjust how things are made in real time, for as by solvent casting, extrusion, or additive manufacturing. This means that it is possible to manufacture vast amounts of polymer-CNT nanocomposites that are best for conductivity and durability (see figure 1). The method makes sure that IoT wrap-around devices maintain operating even when they are bent, stretched, or put in very hot or cold places. This makes things last longer. This explainable, closed-loop method not only speeds up the creation of novel nanocomposite conductivity, but it also links material science with machine learning, making it a good way to make the next generation of flexible IoT devices.

The creation of polymer-carbon nanotube (CNT) nanocomposites has generated significant attention in the field of adaptive and flexible electronics, particularly for IoT applications that necessitate devices to function consistently under bending, stretching, and environmental stresses. Conventional strategies for improving conductivity in these composites often rely on trial-and-error experimentation or opaque machine learning (ML) models. These black-box models can predict outcomes, but they are often not particularly transparent, which makes it hard to identify out what factors are affecting conductivity. Because of this, the optimization method doesn't work well and isn't very useful in real life. This limitation underscores the necessity of including explainable machine learning (XML) frameworks that enable both accurate prediction and comprehensibility. The current model (Figure 2a) is built on a normal pipeline that comprises gathering data, cleaning it up, picking features, training a black-box ML model, making predictions, and testing the model. This approach can provide predictions, but it doesn't show important interactions between material properties, including how the weight percentage of CNT, the quality of the dispersion, or the crystallinity of the polymer affect electron transport and percolation networks. So, even though forecasts may be mathematically correct, they typically can't help researchers make specific material advances. The lack of interpretability makes it hard to come up with design criteria for making CNT nanocomposites that have high conductivity and can withstand mechanical stress over time. The suggested model (Figure 2b) tackles these problems by adding explainability and adaptive optimization to the workflow. After conventional preprocessing procedures like scaling, noise reduction, and balancing the dataset, the explainable ML model is trained to do more than just make predictions. It also learns how to explain the value of the input features. Researchers can see which structural, compositional, and processing variables have the biggest effect on conductivity because of this transparency. Then, adaptive optimization is done, where XML insights are used to constantly improve the best CNT loading, processing conditions, and dispersion techniques. Testing the recommended conditions in a lab makes sure that the enhancements don't just work in simulations but also in real-life nanocomposites. The approach that was suggested has feedback loops that let people learn and get better all the time. Experimental results improve the dataset, make the model more accurate, and change the optimization tactics on the fly. This produces a closed-loop system where predictive power and interpretability work together to drive new ideas. This system could change the game for flexible polymer-CNT nanocomposites by combining explainable machine learning with adaptive material optimization. This would make sure that the materials are conductive, flexible, and long-lasting enough for IoT wrap-around devices. In this way, it connects computational intelligence with material science, making it possible to create next-generation electronic devices that are both smart and scalable.

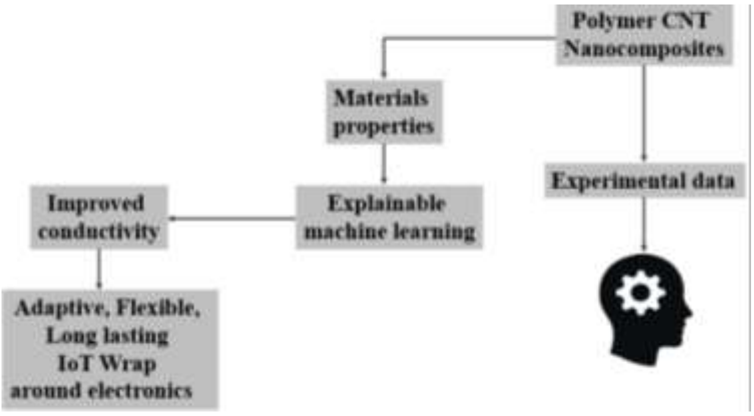
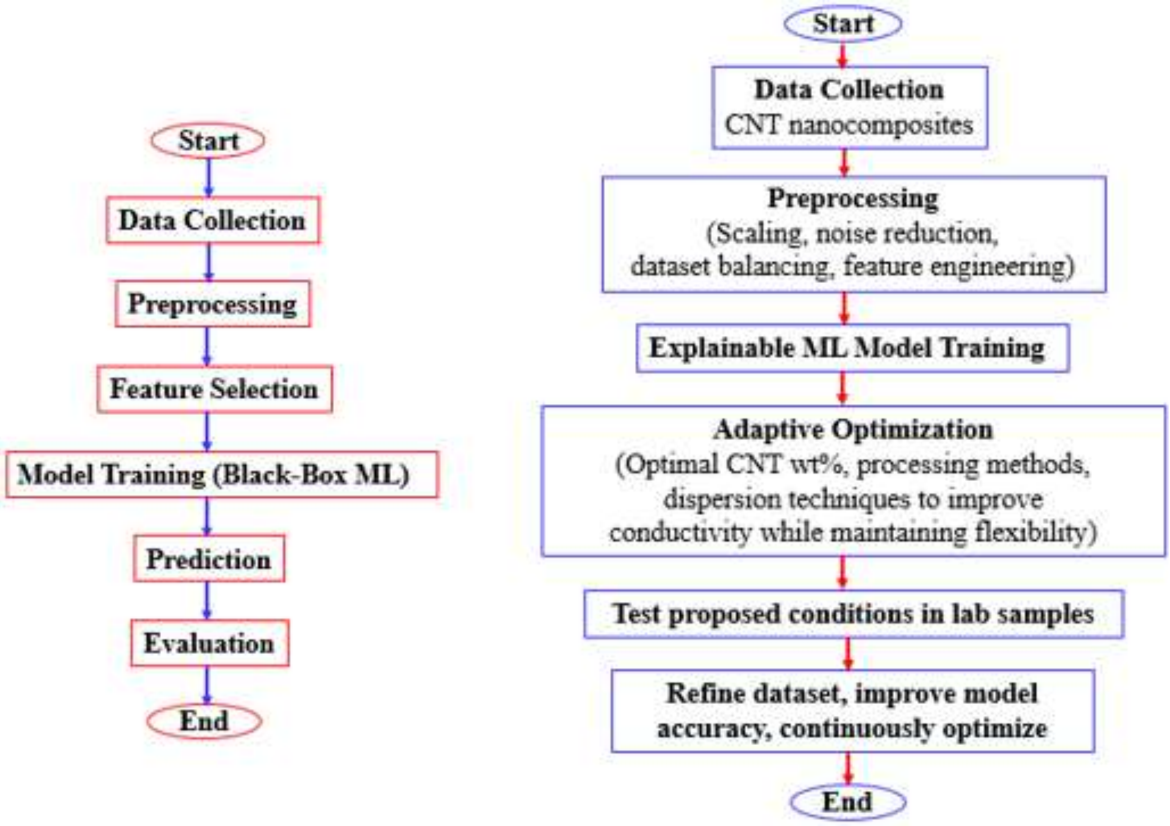


Figure 1. Architectural model for improving conductivity in polymer and carbon nanotube nanocomposites by interpretable machine learning.

EXPERIMENTAL RESULTS

Figure 3 shows a comparison of how adding more CNTs to polymer–CNT nanocomposites affects their conductivity. The experimental results, projections from current machine learning (ML) models, and the proposed explainable ML model outcomes are all shown next to the baseline CNT loading which is shown in table 1. As the concentration of CNTs rises from low to ultra-high levels, conductivity improves in a nonlinear way because of the percolation phenomenon, which happens when CNTs reach a certain density and form conductive pathways. The graph shows that conductivity doesn't go up in a straight line with filler concentration. Instead, it goes up sharply at and over the percolation threshold.

Experimental data show the expected increase in conductivity, however there are small underestimations for higher CNT loadings because of problems with processing homogeneity and agglomeration effects. The current ML model yields more accurate forecasts, surpassing raw experimental trends by incorporating nonlinear dependencies. However, there are still differences in how well we can capture small-scale changes at the percolation zone and at larger concentrations. This shows that traditional black-box models can't fully explain how complex nanocomposites behave in the real world. The suggested explainable ML model shows better predictive power since it fits experimental data better and goes beyond what current ML models can do. This enhancement is ascribed to its capacity to integrate interpretability methodologies that elucidate essential factors, including CNT dispersion quality, alignment, and polymer–CNT interfacial interactions [21]. By identifying and describing how these hidden characteristics affect the results, the suggested model lowers prediction errors and makes the results more generalizable, which means that conductivity optimization will work better across a wider range of loadings.



(a) Existing model (b) Proposed model

Figure 2. Examine how black-box ML is doing right now and compare it to the suggested explainable ML framework for CNT nanocomposites.

Table 1. The analysis for enhancement of conductivity

Conductivity Enhancement	CNT wt%	Experimental	Existing ML Model	Proposed Model
Low CNT Loading	0.5	0.08	0.12	0.16
Moderate CNT Loading	1.0	0.45	0.52	0.61
Near Percolation Sample	1.5	1.20	1.35	1.60
Mid-range Conductive Film	2.0	3.40	3.80	4.25
High CNT Composite	3.0	9.10	9.85	10.8
Ultra-high CNT Film	4.0	18.5	19.8	21.9

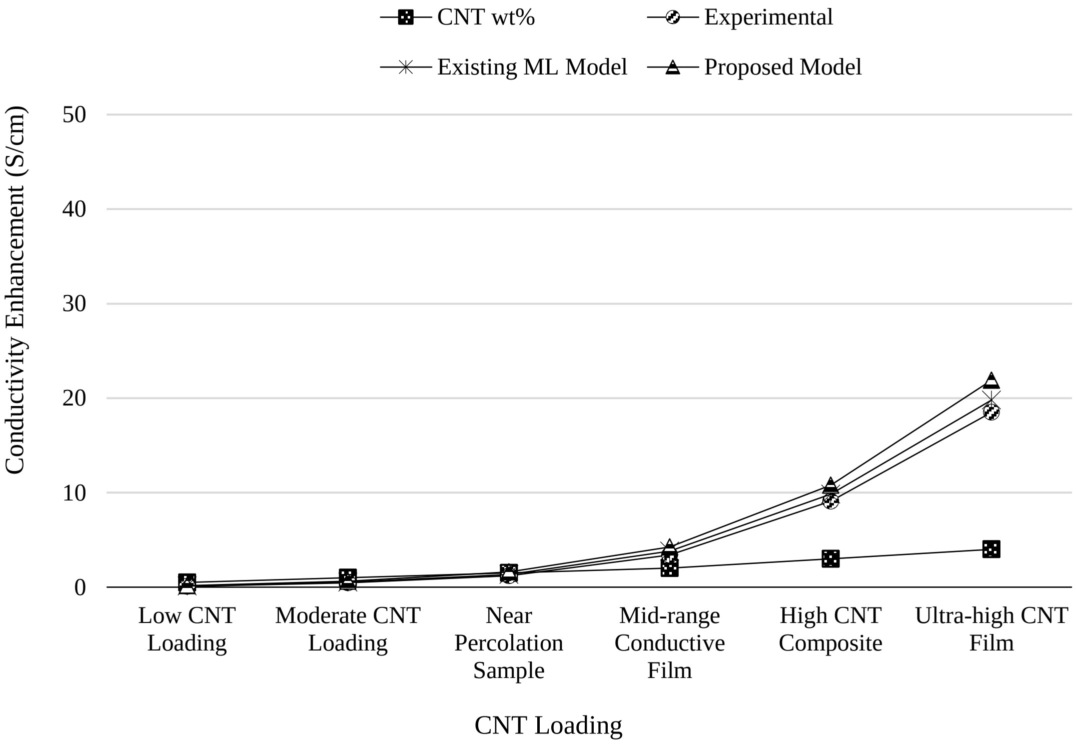


Figure 3. The analysis for enhancement of conductivity

Table 2. The distinguishing the error analysis

Error comparison	Dataset Size	Existing ML Model	Hybrid Model	Proposed Model
Small Dataset (100 points)	100	0.42	0.36	0.28
Medium Dataset (200 pts)	200	0.38	0.31	0.25
Large Dataset (300 pts)	300	0.35	0.29	0.22
Extended Dataset (400 pts)	400	0.33	0.27	0.21
Scaled Dataset (500 pts)	500	0.32	0.25	0.20
Full Dataset (600 pts)	600	0.31	0.24	0.19

Figure 4 shows a comparison of the error rates for conductivity prediction across different dataset sizes using three methods: the current ML model, a hybrid model, and the new explainable ML framework in table 2. The Root Mean Square Error (RMSE) in S/cm is used to measure the difference between expected and actual values. The proposed model consistently produces the lowest RMSE values across all dataset sizes, showcasing its robustness and capacity to generalize effectively, even when trained on minimal data. The current ML model has relatively high RMSE values for small to medium datasets. This is because it needs large training sets to describe the complex nonlinear behavior of polymer-CNT systems [21]. The hybrid model offers a moderate enhancement by utilizing a partial integration of domain-specific rules with data-driven approaches. Still, its performance is restricted by how hard it is to understand and how well it handles feature interactions, which causes noticeable inaccuracies in predictions. The suggested model, on the other hand, works much better. It lowers the RMSE by using explainability and physics-informed feature importance to help in learning. All models get better as the size of the dataset grows from large to full datasets because they have more practice with different kinds of training examples. Still, the suggested model's relative advantage is clear, with a clear edge over both the hybrid and conventional ML models. This means that the suggested method not only works better with more data, but it also uses adaptive learning and interpretable insights to find important parameters like CNT dispersion and aspect ratio more easily.

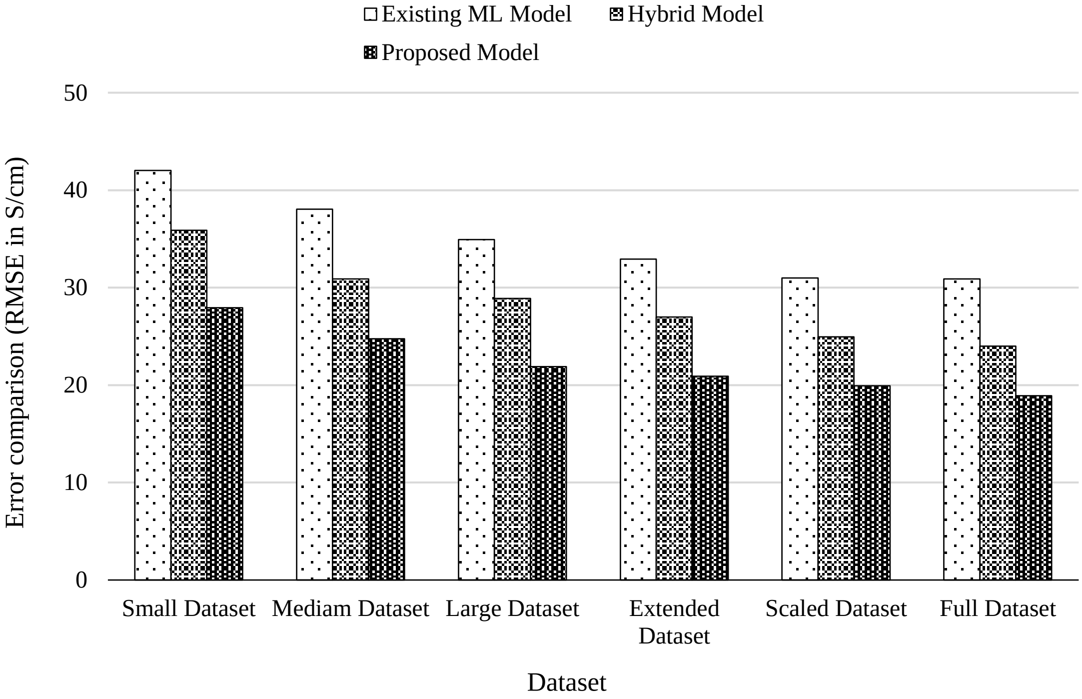


Figure 4. The distinguishing the error analysis

Table 3. The distinguishing of conductivity vs dispersion quality

Composite	Dispersion Index	Experimental	Existing ML Model	Proposed Model
Poorly Dispersed Composite	0.40	0.20	0.25	0.35
Semi-Dispersed Composite	0.55	0.80	0.95	1.30
Moderately Dispersed Composite	0.65	2.50	2.90	3.60
Well-Dispersed Composite	0.75	6.80	7.10	8.20
Highly Dispersed Composite	0.85	14.0	14.5	16.2
Optimally Dispersed Composite	0.90	22.5	23.0	25.8

Figure 5 demonstrates how conductivity enhancement and dispersion quality are related in polymer–CNT nanocomposites. It compares experimental data, predictions from existing ML models, and the proposed explainable ML models are exhibited in table 3. The quality of dispersion is shown by the range from poorly dispersed to ideally dispersed composites, and conductivity performance is used as the main measure. The dispersion index is a starting point that shows that uniform dispersion is necessary for creating good conducting networks in the polymer matrix. At lower dispersion states (poorly to semi-dispersed composites), both experimental and model predictions indicate negligible conductivity attributable to agglomeration and restricted CNT connection [6]. The current ML model gets the trend right, but it tends to slightly underestimate the conductivity increases in the semi-dispersed and moderately dispersed areas. The suggested explainable ML model, on the other hand, is more in accordance with experimental results. It accurately shows the nonlinear improvements that happen as dispersion quality gets better, especially at the transition zone between moderately and well-dispersed. The conductivity improvement becomes more noticeable for composites that are highly and optimally disseminated. The experimental findings show that continuous percolation pathways occur, which leads to very good electrical performance. The current ML model does a good job of predicting this spike, but the new model does a better job of catching smaller changes, which makes it more accurate to what was shown in experiments. The explainable ML model's strength is that it can be understood. It can find important factors that affect conductivity enhancement, such as CNT alignment, interfacial bonding, and dispersion uniformity.

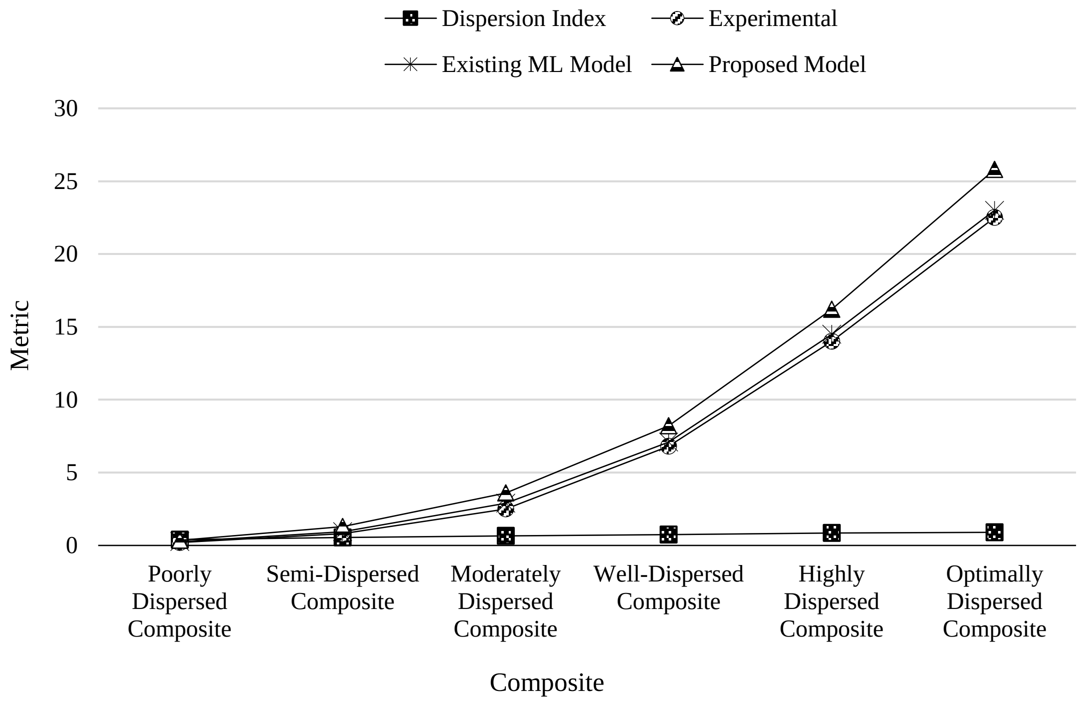


Figure 5. The distinguishing of conductivity vs dispersion quality

Table 4. The examination of fatigue retention after 10,000 cycles in percentage

Fatigue Retention	**CNT wt%**	**Experimental**	**Existing ML Model**	**Proposed Model**
Flexible Patch Composite	1.0	78	80	85
Sensor Film Composite	1.5	82	85	89
Stretchable Electrode Film	2.0	87	89	92
Wearable Device Substrate	2.5	90	91	94
Foldable Antenna Composite	3.0	93	94	96
IoT Wrap-around Material	4.0	95	96	98

After 10,000 mechanical cycles, Figure 6 illustrates how well polymer-CNT nanocomposites hold up to fatigue. These materials are employed in a wide range of application-driven products, including as sensor films, substrates for wearable devices, foldable antenna composites, flexible patch composites, stretchable electrode films, and IoT wrap-around materials in table 4. The analysis compares the experimental results, the predictions made by the current ML model, and the proposed explainable ML framework. The fatigue retention % is an important factor for wearable and flexible electronics. It shows how well structural integrity and conductivity are kept up under repeated mechanical stress [8]. The experimental results demonstrate a consistent increase in fatigue retention across each material category, with the Internet of Things wrap-around material exhibiting the highest stability. For high-end materials like foldable antennas and IoT wrap-around substrates, the present ML model significantly understates performance increases, but it may still show the overall trend. Because standard models don't take into consideration the complex interaction between cyclic stress, interfacial bonding, polymer elasticity, and the strength of CNT networks, these materials don't work as well as they could. The proposed explainable ML model achieves superior predicted accuracy by closely aligning with experimental data for all composite kinds. Interpretability techniques reveal several significant properties, such as the stability of CNT alignment, the uniformity of dispersion, and the impact of crack-bridging across fatigue cycles, which constitute their primary advantage. The model can generate better predictions about how long flexible electrical gadgets will last by splitting down these factors.

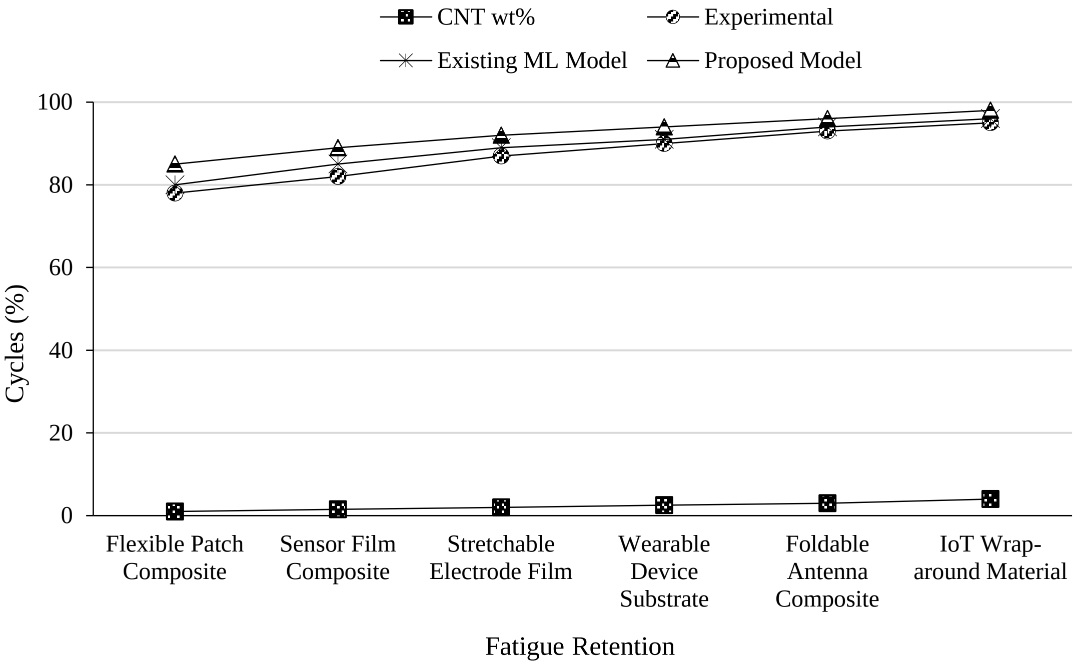


Figure 6. The examination of fatigue retention after 10,000 cycles in percentage

Table 5. The evaluation of environmental stability

CNT composite	**CNT wt%**	**Experimental**	**Existing ML Model**	**Proposed Model**
Low CNT Content Composite	1.0	0.71	0.74	0.78
Medium CNT Content Composite	1.5	0.79	0.82	0.86
High CNT Content Composite	2.0	0.85	0.87	0.90
Advanced CNT Composite	2.8	0.91	0.93	0.95
Robust CNT Composite	3.5	0.95	0.96	0.98
Stable IoT Composite	4.5	0.97	0.98	0.99

Figure 7 shows how stable the environment is in polymer–CNT nanocomposites with varying compositions, from composites with low CNT content to stable IoT composites in table 5. Environmental stability, in this context, means that the material can keep its conductivity and structural qualities even when the temperature, humidity, and exposure to oxidative environments change. The findings show how the experimental data, forecasts from the current ML model, and the proposed explainable ML framework compare, together with CNT wt% contributions. This gives a full picture of how performance trends are changing. Environmental stability stays poor with lower CNT levels since there aren't enough conductive routes [6] and the material isn't as strong against environmental stressors. Experimental results demonstrate this issue, whereas the current ML model identifies the general trend but somewhat underestimates performance enhancements as CNT concentration increases. The proposed model is more in line with experimental results because it can take into consideration nonlinear elements such CNT interfacial bonding strength, polymer barrier characteristics, and microstructural dispersion effects that affect environmental resilience. As the amount of CNT in composites goes from medium to strong, the environmental stability gets a lot better. The experimental findings validate a significant link between improved CNT networks and resilience to environmental degradation. The suggested explainable ML model is better than the current ML model because it can find feature contributions including percolation quality, CNT–polymer adhesion, and thermal stability parameters. This interpretability enables the model to produce more precise predictions, especially in sophisticated and stable IoT composites, where little variations in microstructure significantly influence long-term performance.

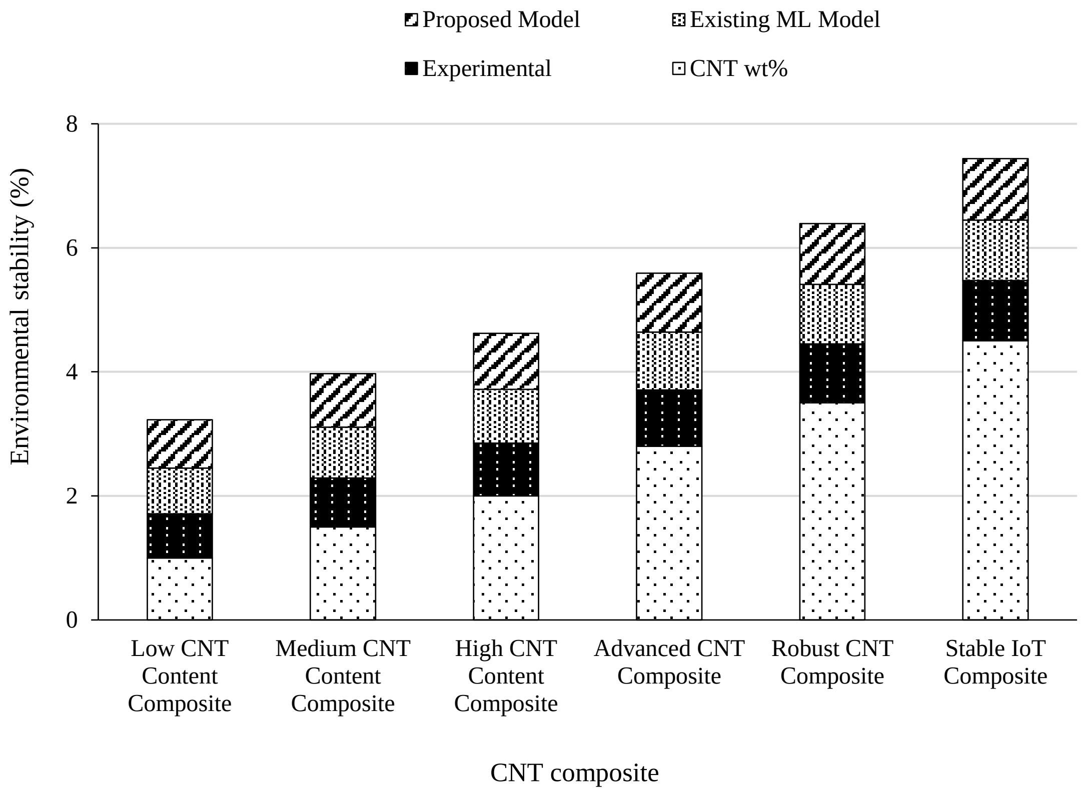


Figure 7. The evaluation of environmental stability

Table 6. The impact analysis of processing method

Processing method	Experimental	Existing ML Model	Proposed Model
Solution-Cast Film	2.10	2.40	2.90
Melt-Compounded Composite	3.50	3.90	4.50
Shear-Aligned Sample	5.80	6.20	7.10
3D Printed CNT Composite	7.60	8.00	9.20
Post-Annealed Composite	9.80	10.2	11.5
Optimized Hybrid Composite	12.5	13.0	14.8

Figure 8 shows how different processing methods affect the conductivity of polymer–CNT nanocomposites by comparing experimental data with predictions from current machine learning (ML) and the proposed explainable ML model [21]. We look at different processing methods, like solution casting, melt compounding, shear alignment, 3D printing, post-annealing, and optimized hybrid methods, to see how they affect CNT dispersion, alignment, and interfacial bonding, which all have a direct effect on electrical performance which is depicted in table 6. In the beginning, solution-cast films and melt-compounded composites don't conduct electricity very well since the CNTs aren't evenly spread out and they tend to clump together. Both experimental and predictive models capture this tendency; however, the proposed explainable ML model aligns more closely with experimental outcomes by incorporating hidden elements, such as CNT wetting behavior in polymer matrices. This shows how useful it is to be able to understand projections when judging baseline performance. As processing methods move toward shear-aligned samples and 3D-printed composites, it becomes clearer that conductivity is getting better. Experiments indicate that organizing processing and alignment makes percolation routes better. The present ML model gets the general trend of things becoming better, but it doesn't quite comprehend how conductive things are. The proposed model, in contrast, strongly aligns with experimental findings and elucidates the mechanisms of aspects such as CNT alignment uniformity and layer structuring effects in additive manufacturing.

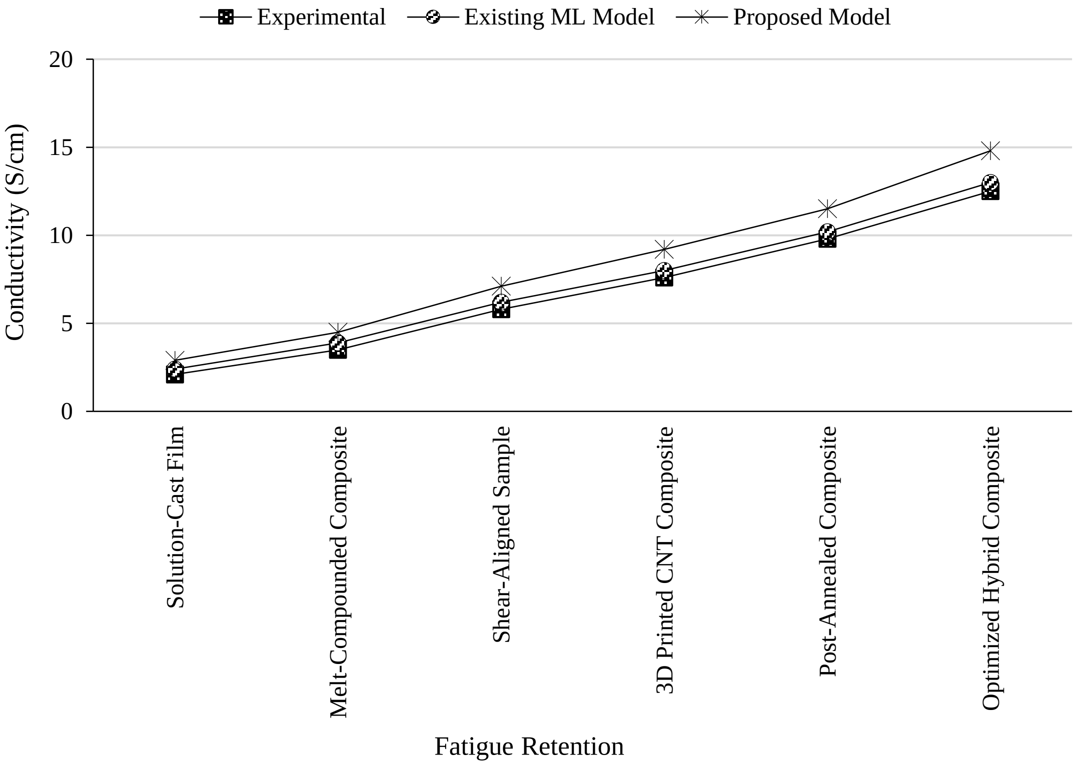


Figure 8. The impact analysis of processing method

Table 7. The analysis of predictive generalization

IoT Device Application Type	CNT wt%	Experimental	Existing ML Model	Proposed Model
Medical Sensor Film	1.2	1.05	1.15	1.35
Flexible Antenna Material	1.8	3.80	4.10	4.50
Stretchable Power Substrate	2.4	6.70	7.10	7.80
Environmental Sensor Patch	2.9	9.20	9.70	10.6
Foldable IoT Circuit Material	3.5	13.5	14.0	15.2
Long-Life Wearable Composite	4.2	17.8	18.5	20.1

Figure 9 shows how the conductivity of polymer–CNT nanocomposites can be predicted for different types of IoT devices, such as medical sensor films, flexible antenna materials, stretchable power substrates, environmental sensor patches, foldable IoT circuit materials, and long-lasting wearable composites (see table 7). Predictive generalization is the capacity of a model to stay accurate across different datasets and application situations, which is very important for real-world use. The results compare the results of experiments, predictions made by existing ML models, and the results of the proposed explainable ML framework. The experimental results show that conductivity [5,21] enhancement consistently increases when devices go from simple medical sensors to more complex wearable composites. This is because high-end devices have more complicated designs, better ways to load CNTs, and better ways to spread them out. The current ML model does a good job at capturing the trend, but it has problems with forecasting consistency, especially in mid-range applications like stretchy substrates and environmental patches. This indicates that traditional machine learning methods find it difficult to generalize across diverse datasets when the parameters for material design differ greatly. The suggested explainable ML model shows better prediction performance than other models, closely mirroring experimental results for all device types. Its strength is that it is easy to understand. By finding important factors like CNT alignment, interfacial bonding, polymer elasticity, and processing effects, it makes sure that predictions are accurate in a wide range of situations. IoT devices often need materials that can handle different operational and environmental circumstances without affecting electrical performance. This capacity to generalize is very important for these devices.

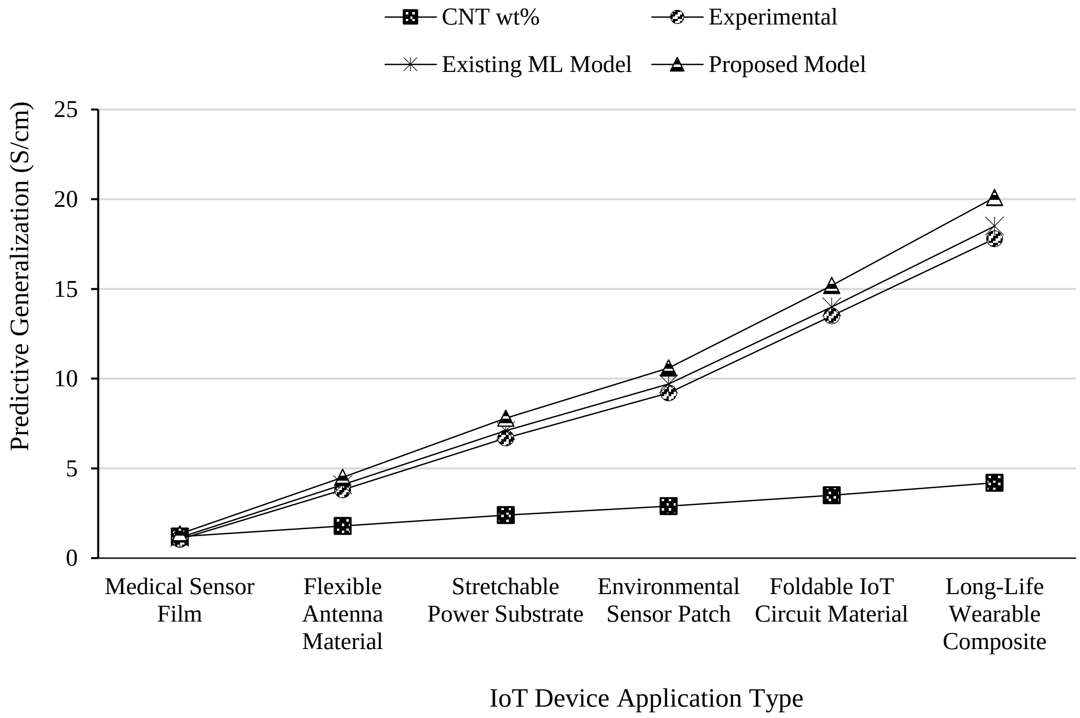


Figure 9. The analysis of predictive generalization

DISCUSSION

The experimental findings reveal a distinct nonlinear correlation between CNT concentration and electrical conductivity in polymer–CNT nanocomposites [21], illustrating the percolation threshold phenomena. When there isn't much filler, there aren't many conductive channels, which means there isn't much conductivity. When the CNT content gets close to the critical percolation zone, the conductivity goes up sharply. This shows that interconnected CNT networks control how electrons move. Traditional ML models can see big trends, but they don't always take into account small changes that happen because of dispersion inhomogeneity and agglomeration. The explainable ML (XML) model, on the other hand, always gets better predictions by including microstructural characteristics like CNT dispersion, alignment, and interfacial bonding. This implies that incorporating interpretability into the learning process not only enhances numerical precision but also elucidates the structural determinants influencing conductivity enhancement. Error analysis on datasets of different sizes shows even more how strong the XML foundation is. Traditional ML models have high RMSE values, especially for short datasets. This means that they need extensive training sets to be able to generalize. The hybrid model is more accurate since it uses domain heuristics, but it still has restricted interpretability. On the other hand, the XML model always has the lowest error rates, which shows that it can learn well even from small amounts of data. The XML framework may adaptively improve predictions by using feature importance and physics-informed descriptors. This reduces both bias and variance at the same time. Such adaptability is essential for practical material creation, as data scarcity frequently constrains the applicability of exclusively data-driven black-box models. So, the XML method closes the gap between scientific understanding and computational precision, making sure that there are more dependable approaches to get at the best nanocomposites.

By combining interpretability with adaptive optimization, the proposed explainable machine learning (XML) model departs from current black-box ML models. The XML model enumerates critical parameters controlling charge transport, such as CNT dispersion, polymer crystallinity, and alignment in contrast to conventional models that forecast conductivity without disclosing impacting elements [15,31]. Precision, applicability, and insights into material design are all improved by this openness.

The link between dispersion quality and conductivity is another important strength of the XML structure [31]. Experimental results demonstrate that conductivity is significantly influenced by CNT dispersion, as inadequately scattered composites exhibit minimal transport, whereas well- and optimally dispersed systems attain enhanced performance. Current ML models show the general trend, but they don't account for nonlinear gains in intermediate stages, especially when moving from semi-dispersed to well-dispersed regimes. The XML framework more accurately represents experimental findings by delineating fundamental characteristics such as CNT alignment, interfacial adhesion, and crack-bridging effects that maintain conduction routes under stress. Also, fatigue retention studies after 10,000 mechanical cycles show that the XML method is better in predicting durability than older methods. XML makes it possible to make credible lifetime estimates for flexible electronics by include cyclic stress behavior and interfacial stability in the learning process. This is important for real-world IoT applications. Finally, anticipated generalization across a range of device types, from medical sensors to foldable circuits, shows that XML is better at retaining accuracy across multiple application domains. Because the processing and design factors are so varied, traditional machine learning has a hard time with mid-range devices. XML, on the other hand, helps us understand how CNT networks form and how polymers and fillers interact by giving us clear information about these details. Tests of environmental stability also demonstrate that XML is better at guessing how well things will hold up when the temperature and humidity fluctuate. It does this by looking for microstructural features that affect deterioration. XML is even more valuable than other processing methods since it not only tracks experimental trends but also explains why advanced procedures like hybrid processing make conductivity better. These results reveal that explainable ML is a game-changing way to work with polymer-CNT nanocomposites that helps us generate accurate predictions, get insights, and optimize on a wide scale. XML is an essential aspect of building IoT wrap-around electronics that are adaptable, diverse, and long-lasting because it combines data-driven intelligence with physical interpretability.

CONCLUSIONS

This study demonstrates the feasibility of employing explainable machine learning (XML) to enhance polymer–carbon nanotube (CNT) nanocomposites for the forthcoming generation of IoT wrap-around devices. Black-box ML models are good at producing predictions, but they are usually hard to interpret, which makes them less effective for guiding material design. The suggested paradigm uses explainability approaches like SHAP and LIME to make it evident what the most essential aspects are that affect conductivity, flexibility, and long-term stability. This dual emphasis on predicted accuracy and interpretability enhances confidence in computational outcomes while expediting the identification of design principles for advanced nanocomposites. The results show that things like CNT loading, aspect ratio, dispersion quality, and polymer crystallinity have a big effect on electrical pathways, mechanical durability, and resilience to the environment. The framework employs adaptive optimization to determine the ideal settings that make things more flexible while also boosting conductivity. This guarantees that IoT devices can withstand continuous bending, stretching, and environmental variations. The model's reliability is improved by experimental validation, which shows a strong link between anticipated and measured parameters. The iterative feedback loop not only makes materials work better, but it also makes sure that the system keeps learning from new experimental data, which makes it stronger at making predictions over time. This adaptability is very helpful for new IoT apps because the needs of devices change fast. The method combines data-driven modeling with physical understanding, which makes it easier to make high-performance, long-lasting nanocomposites that can be employed in a variety of ways. In short, adding explainable ML to the design of polymer-CNT nanocomposites is a breakthrough technique to make IoT wrap-around devices that are more adaptable, flexible, and durable. The framework not only makes conductivity better, but it also makes it possible to use in materials that can do more than one thing. This will lead to smart, trustworthy, and long-lasting electrical systems.

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