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Machine Learning Based Optimization of Polymer Structure Property Relationships in Composite Material Systems

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Abstract

In modern engineering applications, polymer-based composite materials have garnered a lot of attention because of their lightweight nature, high strength-to-weight ratio, and changing physical features. In order to maximize the relationships between polymer structure and properties in composite materials, this study suggests a strategy based on reinforcement learning (RL). The research utilized the Polymer Composite Properties Dataset, which contains 12,700 records associated with polymer matrices, reinforcement fillers, interfacial bonding characteristics, curing conditions, thermal properties, processing variables, and mechanical performance indicators. To ensure accurate representation of structure–property correlations, material characterization was carried out using X-ray diffraction (XRD) for phase identification, Fourier transform infrared spectroscopy (FTIR) for chemical interaction analysis, and scanning electron microscopy (SEM) for microstructural analysis. Tensile strength, elongation at break, Young's modulus, impact toughness, and other mechanical parameters were tested in accordance with the American Society for Testing and Materials (ASTM) recommendations. Thermal stability was assessed by thermogravimetric analysis (TGA). A deep Q-network (DQN)-based RL agent was used to repeatedly modify polymer structural properties, such as chain design, crosslink density, and filler dispersion. The agent was guided by reward functions derived from surrogate models trained on the experimental dataset. The model achieved minimum MSE values of 0.0478, 0.3520, 0.0857, and 3.5042, along with MAE values of 0.1850, 0.5017, 0.2694, and 1.5607, respectively, confirming its superior capability in capturing nonlinear structure–property relationships of polymer composites (PC). The results demonstrate the capability of RL to capture complex nonlinear interactions, accelerate the design of high-performance PC, reduce experimental effort, and enable efficient material innovation.

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INTRODUCTION

Composite materials formed from polymers have been widely used owing to their properties of light weight, high durability, and resistance to heat and

corrosion. Polymer composite materials have been widely applied in sectors like aviation, automotive, medical sciences, construction, and energy, where performance optimization is crucial [1, 2]. The performance of polymer composite materials is mostly reliant on the structure-property relationship that refers to the effect of molecular structure, filler composition, reinforcing materials, and processing conditions on material properties like tensile strength, elasticity, conductivity, resilience, and heat resistance. However, determining the best polymer structure to attain specific material properties is a challenging task [3, 4].

Conventional techniques to design polymers and optimize composites are predominantly dependent on trial-and-error experimentation, computer simulations, and statistical models. Even though these techniques offer useful information, they are costly and time-intensive, especially when there are many design possibilities and several objective functions [5, 6]. Furthermore, ML algorithms have demonstrated significant promise in material property prediction; nevertheless, they lack the flexibility required to make decisions regarding the optimization of the polymer's structure. This is why autonomous intelligent optimization systems have been designed to explore the space of materials and improve their performance [7, 8].

RL, which is one of the artificial intelligence techniques, can be seen as a solution methodology for tackling difficult optimization problems by interacting with the environment [9]. Contrary to supervised learning approaches, RL systems can adaptively and sequentially select action choices depending on whether the system receives a reward or penalty due to the choice made. Therefore, in the case of polymer composite materials, RL systems can be used to optimize the molecular structure, reinforcement material, filler, and process parameters to match specific material characteristics [10, 11].

The recent developments in the field of deep RL, generation models, and materials science based on big data have additionally increased the potential of optimization using the principles of RL in the context of material engineering [12]. With these techniques, one can automatically explore the wide range of possibilities that are available when designing polymers, predicting the relation between structure and properties of materials, and determining the best composite formulation, thereby resulting in materials that exhibit excellent mechanical, thermal, and electrical performance. Multi-objective optimization can also be applied here, considering different parameters such as durability, strength, sustainability, and cost [13, 14].

Research aim and organization

The objective of the research is to design an RL-based framework for the optimization of polymer composite materials in terms of their property-structure relations through the enhancement of polymer structure, filler, and processing parameters for improved mechanical and thermal properties.

The structure of the research is as follows: An introduction is given in Section 1; a review of the literature is given in Section 2; Materials and dataset preparation for experimentation are presented in Section 3; Section 4 discusses the RL method to predictive maintenance; Section 5 presents results and discussions; and Section 6 gives conclusion.

PREVIOUS RESEARCH

Table 1 reviews recent studies on ML–based prediction and optimization techniques for polymer composite materials, highlighting their methodologies, key findings, and existing limitations.

MATERIALS AND EXPERIMENTAL DATASET PREPARATION

The selection of fillers, polymers, and additives used to create PC is covered in detail in this section. Data pertaining to the preparation and analysis of the experimental dataset is also included in this part. SEM, XRD, FTIR, TGA, and ASTM tests were performed on PC to provide an experimental dataset with 12,700 observations.

Table 1. Overview of recent research on ML applications in PC.

Ref.	Aim	Method/data	Key results	Limitation
[15]	Develop hybrid natural fiber composites and predict properties using ML.	Hand lay-up fabrication, FTIR, dynamic mechanical analysis (DMA), TGA, Random Forest [RF], Atomic force microscopy (AFM).	Tensile strength 85.8 MPa; RF achieved R^2 up to 0.968.	Small dataset and lab-scale study.
[16]	Optimize compressive strength of Polylactic Acid composites using ML.	Six ML models with Fused Filament Fabrication printing parameters and SHapley Additive exPlanations (SHAP) analysis.	Polynomial Regression achieved $R^2 = 0.88$ with 3.44% error.	Limited parameters and a specific Polylactic Acid system.
[17]	Estimate how fused deposition modeling polymer composites behave mechanically.	Bayesian linear regression, Box–Behnken design, Analysis of variance, and Gaussian process regression models.	Gaussian process regression achieved an R^2 above 0.99 with low error.	Limited material combinations and conditions.
[18]	Review ML applications in PC.	Literature survey on ML-based prediction and optimization.	ML improved the prediction and optimization of composites.	No experimental validation.
[19]	Predict properties of P3HB nanocomposites using ML.	SEM characterization with RNN, DT, RF, and RNN-LV models.	Stiffness improved by 132%; best test $R^2 = 0.9203$.	Limited filler combinations and industrial validation.

Dataset Construction

There are 12,700 data entries in the database about polymer-based composite materials used in engineering. This data set's aim is to determine the connections between the polymer architectures, filler material properties, processing parameters, micromechanical properties, thermal behavior, and mechanical behavior of the composite materials. Polymer matrixes, filler material, interface interaction, process parameter, thermal behavior, and optimization parameters of the reinforcement of the composite materials are included in the data set. (https://www.kaggle.com/datasets/colabsss/polymer-composite-properties-dataset)

Material Selection

Diverse polymers matrix, reinforcements fillers, and processing aids were selected for designing varied composite structures. Thermoplastics and thermoset polymers matrices, including polyethylene (PE), polypropylene (PP), polyamide (PA), epoxy resin, and polyester resin, were selected owing to their mechanical strengths and processability. Graphite fiber, carbon fiber, graphene nanoparticle, silica nanoparticle, and carbon nanotube (CNT) were used as reinforcements to enhance strength and thermal stability. Processing aids like coupling agent, curing agent, plasticizer, and stabilizer were added to promote interfacial interaction, plasticity, curing reaction, and thermal stability.

Composite Fabrication

Polymer composites were synthesized by implementing controlled mixing, dispersion, and curing steps to provide uniform filler distribution and uniform material behavior. Polymer matrices and reinforcing fillers were mixed by means of mechanical stirring and ultrasonication to minimize filler agglomeration and enhance filler-matrix interface interactions. Coupling agents and curing agents were added to the composite formulations during synthesis. Fabrication was done using compression molding, casting, and hot pressing methods at appropriate temperatures and pressures. Curing was done for thermosetting composites in programmed ovens. Lastly, samples were cut, polished, cooled, and machined following ASTM specifications.

Experimental Characterization

The morphological, structural, mechanical, and thermal characteristics of the produced PC were examined through experimental investigations. The material's shape was examined using SEM, its structure and chemistry were characterized using XRD and FTIR, mechanical testing that complied with ASTM standards was carried out, and thermal analysis was done using TGA.

Morphological Analysis

SEM analysis was used to research the surface dispersion, morphology, and binding characteristics of fillers present in the developed polymer composite materials. The results from the SEM analysis gave many important details about the filler dispersion, fracture behavior, and matrix-filler interactions.

Structural and Chemical Analysis

The phases, fillers distribution, and structure of the composite materials in question have been analyzed using the XRD analysis technique. The XRD results have shown all the characteristics pertaining to phase composition, crystallinity, and other structural elements influencing the mechanical and thermal properties of the polymer composite materials. The size of the crystallites has been calculated from Scherrer's equation:

$$n\lambda = 2d \sin\theta \tag{1}$$

In Equation (1), θ is the diffraction angle of the X-ray beam, d represents the interplanar distance between crystal planes, the wavelength of the incident X-ray is indicated by λ, and the order of diffraction is denoted by n.

The interaction studies in the composite material were performed by FTIR spectroscopy. Through the observation of the absorption peaks, the FTIR spectroscopy was helpful in detecting the interface interaction of the polymer matrix and the reinforcing particles. The test would be able to provide useful data regarding the interaction, such as the formation of chemical bonds and cross-links. The transmittance equation of the FTIR test is shown below:

$$T = \frac{I}{I_0} \tag{2}$$

In Equation (2), I is the intensity of light transmitted, T represents transmittance, and I_0 is the incident light intensity. The above analysis was useful in determining bonding and interactions at interfaces in the polymer composite system.

Mechanical Property Evaluation

ASTM guidelines were used to examine the composite material's mechanical characteristics. The purpose of the tensile test was to determine the highest tensile stress that the composite could withstand before failing. To ascertain the material's elastic characteristics, the Young's modulus test was performed. The elongation at break test was used to assess the composite's flexibility. The ability of the material to withstand energy impact without cracking was evaluated by an impact toughness test.

Thermal Stability Analysis

The method of TGA analysis was applied to assess the thermal stability and degradation of the composite materials. The weight loss of the composite material at elevated temperatures was measured by this method to determine the breakdown point and thermal stability of the samples. Data collected from the TGA analysis helped in understanding the influence of reinforcement on the thermal stability of the samples

PROPOSED RL METHOD FOR POLYMER COMPOSITE OPTIMIZATION

The recommended RL-based algorithm will apply the DQN to optimize the relationship between structure and properties of the composite polymers taking into account the complicated relationships among the polymer matrices, the filler, and the process parameters. The RL system fine-tunes the parameters of the process, such as the concentration of the filler, cross-link density, and curing temperature.

DQN Agent

A deep RL approach with DQN has been applied to maximize the effectiveness of structure-performance relationships in PC. Traditional optimization procedures can be ineffective in solving

complex problems associated with multi-dimensional and non-linear relations among polymer matrices, reinforcing fillers, manufacturing conditions, and physical properties of the material. To solve the above-mentioned problems, an enhanced DQN algorithm employing a Deep Neural Network (DNN) for approximating the Q-value function was suggested.

The suggested DQN approach assumed that the RL agent was in continuous interaction with the composite material environment via actions associated with structural parameters of the polymer matrices, such as concentrations of reinforcement particles, cross-linking density, curing temperature, and their distribution in the material. To maximize the reward signal corresponding to mechanical strength and thermal stability, experience replay memory and a target network have been introduced into the learning process. The Q-value function in the DQN model was represented using the Bellman optimization principle as:

$$P(l, b) = R + \mu\, P^*(l', b') \tag{3}$$

In Equation (3), R denotes the immediate reward, and μ is the discount factor controlling future rewards. The term $P^*(l', b')$ indicates the optimal future reward for the next state l' and action b'. $P(l, b)$ represents the predicted reward for taking action b in state l. The loss function used for network training was defined as:

$$s(\theta) = \mathbb{E}[(x^{target} - P(l, a; \theta)^2)] \tag{4}$$

In Equation (4), $s(\theta)$ represents the loss value of the neural network, $\mathbb{E}$ denotes the expected average over training samples, x^{target} is the target reward value, and $P\,(l, a; \theta)$ represents the predicted Q-value for state l and action a using network parameters θ. where the target value was calculated as:

$$x^{target} = R + \mu\, max_{b'}(l', b'; \theta') \tag{5}$$

Equation (5) helps the DQN model learn optimal decision-making policies for polymer composite optimization. Algorithm 1 presents the proposed DQN-based RL framework for optimizing polymer composite processing parameters to enhance mechanical and thermal performance through adaptive decision-making.

Algorithm 1: DQN-Based Polymer Composite Optimization

1.Initialize DQN network,target network,and replay memory
2.Observe current composite state l
3.Select action b (adjust filler concentration,curing temperature,crosslink density)
4.Apply action and receive reward R
5.Store transition (l,b,R,l') in replay memory
6.Compute target:
  x_target = R + μ max P(l',b'; θ')
7.Update DQN using loss:
  s(θ) = E[(x_target - P(l,a;θ))²]
8.Repeat until optimal composite performance is achieved

RESULT

The experiments related to the characterization and analysis of the PC prepared using TGA, FTIR, XRD, and SEM methods are discussed in this section. The study examines the prediction efficiency of the RL paradigm used in predicting the properties of polymers using DQN and examines the mechanical and thermal properties of the synthesized PC.

SEM Microstructure of Optimized Polymer Composite with Uniform Filler Dispersion

The findings from SEM analysis demonstrated a good bonding between the reinforcing fillers at their

interface and their uniform distribution throughout the polymer composite material. Further, the microstructure possessed few voids and filler agglomerations, implying proper processing and distribution of fillers in the polymer composite material. It was found that the fracture surface of the specimen was rough in nature, indicating the ability of stress transfer and improved mechanical properties of the polymer composite material in Figure 1.

Structural and Crystalline Analysis of Polymer Composite Materials Using XRD

The XRD method was used to characterize the structure of the PC. The diffraction pattern showed that reinforcing fillers had been successfully added to the polymer matrix. The mechanical and thermal properties of the composite material were improved by higher levels of crystallinity and crystal size (Table 2).

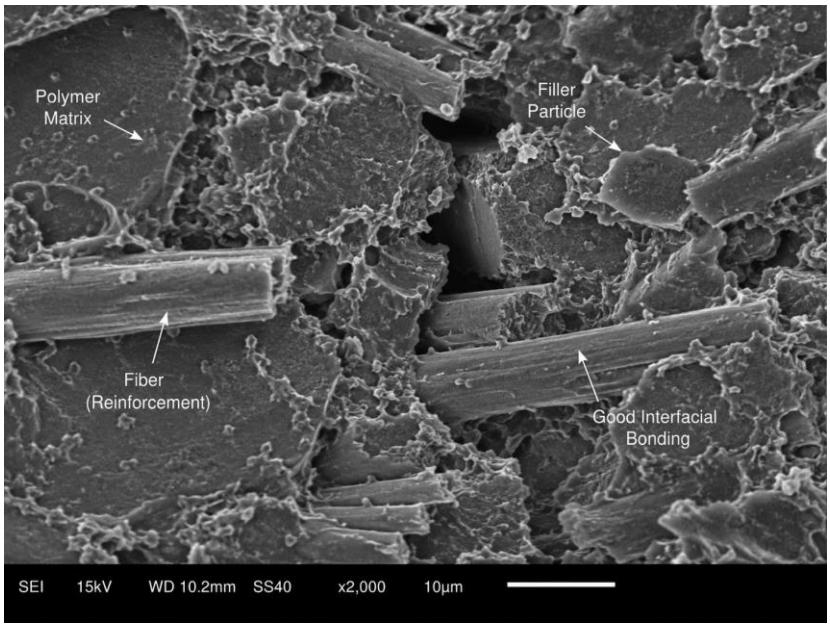

Figure 1. SEM microstructure of reinforcement-enhanced polymer composite.

Table 2. XRD analysis of polymer composite materials.

Sample ID	Polymer matrix	Reinforcement filler	Major diffraction peaks (2θ°)	crystalline Phase identified	Crystallinity index (%)	Average crystallite size (nm)
PC-1	Epoxy	CNT	26.2°, 43.4°	Graphitic Carbon Phase	68.5	24.6
PC-2	PP	Glass Fiber	21.5°, 25.8°	Semi-crystalline PP Phase	61.2	19.8
PC-3	PE	Nano Silica	22.1°, 36.5°	Orthorhombic PE Structure	57.9	17.3
PC-4	Epoxy	Graphene Oxide (GO)	10.8°, 26.5°	GO Layered Structure	72.4	28.1
PC-5	Polyester	Clay Nanoparticles	19.7°, 29.4°	Layered Silicate Phase	64.1	21.5
PC-6	PA	Carbon Fiber	20.3°, 24.1°	α-Crystalline PA Phase	69.7	26.2
PC-7	Vinyl Ester	Aluminum Oxide	35.2°, 43.1°	Alumina Crystalline Phase	66.8	23.4
PC-8	Epoxy	Hybrid CNT/SiO_2	25.9°, 36.2°	Hybrid Reinforcement Phase	74.3	30.6

Table 3. FTIR quantitative analysis of polymer composite materials.

Sample ID	Polymer Matrix	Reinforcement Filler	FTIR Peak Position (cm^{-1})	Peak Intensity (a.u.)	Functional Group	Transmittance (%)	Interpretation
FTIR-1	Epoxy	CNT	3432	0.82	O–H Stretching	71.4	Strong hydroxyl interaction indicating improved filler adhesion
			2924	0.76	C–H Stretching	74.8	Stable polymer backbone structure
			1638	0.69	C=C Bond	78.2	Enhanced CNT dispersion within the matrix
FTIR-2	PP	Glass Fiber	2951	0.73	CH_3 Stretching	76.5	Improved interfacial bonding
			1456	0.65	CH_2 Bending	81.3	Increased structural stability
			1168	0.59	C–O–C Stretch	84.6	Evidence of polymer-filler compatibility
FTIR-3	PE	Nano Silica	1092	0.88	Si–O–Si Stretching	69.2	Strong silica incorporation
			802	0.62	Symmetric Si–O Bond	79.8	Uniform nanoparticle dispersion
			472	0.51	Si–O Bending	86.4	Enhanced inorganic interaction
FTIR-4	Epoxy	GGO	1726	0.91	C=O Stretching	66.7	Oxidized graphene structure confirmed
			1622	0.74	Aromatic C=C	73.9	Improved aromatic interaction
			1228	0.68	Epoxy C–O	77.5	Increased crosslink density
FTIR-5	Polyester	Clay Nanoparticles	1047	0.84	Si–O Stretching	70.1	Layered clay structure is present
			918	0.63	Al–OH Vibration	80.4	Enhanced filler interaction
			3622	0.57	O–H Stretching	85.2	Improved moisture resistance
FTIR-6	A	Carbon Fiber	3302	0.86	N–H Stretching	68.8	Strong amide interaction
			1639	0.78	Amide I Band	72.6	Enhanced tensile reinforcement
			1542	0.71	Amide II Band	76.9	Stable polymer network
FTIR-7	Vinyl Ester	Aluminum Oxide	752	0.55	Al–O Bond	83.7	Alumina reinforcement confirmed
			1086	0.73	C–O Stretching	75.1	Improved matrix rigidity
			3452	0.67	O–H Stretching	78.5	Strong filler-matrix adhesion
FTIR-8	Epoxy	Hybrid CNT/SiO_2	1107	0.93	Si–O–Si Stretching	65.9	Strong hybrid filler interaction
			1580	0.79	Aromatic C=C	71.8	Enhanced conductive network
			3437	0.88	O–H Stretching	69.7	Improved multifunctional properties

FTIR Analysis of Polymer Composite Materials

The identification of the functional groups and the interactions was made using FTIR at a wavelength of 4000 – 400 cm^{-1}. According to Table 3, there are significant peaks for O-H, C=O, N-H, C=C, and Si-O-Si functional groups, which indicate that the reinforcement fillers have been incorporated into the polymer matrix effectively.The intensity of peaks and the variation in transmission indicate effective bonding of the filler and matrix interaction, effective dispersion of the fillers within the matrix, and effective cross-linking.

ASTM Standards for Material Characterization and Testing

ASTM International standards were used in characterization of the PC to ensure accurate results. The mechanical properties of the composites were determined using ASTM D638 and ASTM D256, while thermal stability was measured using ASTM E1131. The morphology of the composites was analyzed using ASTM E2015, structure using ASTM D934, and chemical bonding using ASTM E1252, as shown in Table 4.

Thermal Stability Evaluation Using TGA

The TGA test was based on the ASTM International standards for evaluating the thermal stability of PC. The test was performed under a nitrogen environment from 30°C to 800°C at a rate of 10°C per minute. According to the findings, using CNT, GO, and hybrid filler materials, as well as other fillers, increased the thermal stability of PC (Table 5).

Multivariate Property Analysis and RL Optimization of PC

Figure 2 illustrates the correlation and distribution analysis of the composite properties, namely, crosslink density, crystallinity, thermal conductivity, impact toughness, and glass transition temperature. The results suggest a positive correlation between thermal conductivity and glass transition temperature, as well as a more favorable relationship between impact toughness and thermal conductivity. This indicates the nonlinear relationships among the various composite properties and demonstrates the success of the proposed DQN-based framework for optimization.

Figure 3(a) indicates differences in filler concentration, porosity, cross-link density, and crystallinity in composite specimens. Figure 3(b) shows the distribution of low-performing, mid-performing, and high-performing composites depending on several material parameters. Figure 3(c) displays the variation in Young's modulus, impact resistance, thermal conductivity, tensile strength, and crystallinity of the composites. Figure 3(d) depicts the interconnection between the polymer matrix, filler material, and composite performance classes.

Table 4. ASTM standards used for mechanical and thermal testing.

Test Parameter	ASTM Standard	Purpose of Testing
Tensile Strength	ASTM D638	Evaluation of tensile properties of PC
Young's Modulus	ASTM D638	Measurement of stiffness and elastic behavior
Elongation at Break	ASTM D638	Determination of ductility and deformation capability
Impact Strength	ASTM D256	Assessment of impact resistance and toughness
TGA	ASTM E1131	Evaluation of thermal decomposition and stability
SEM	ASTM E2015	Examination of surface morphology and filler dispersion
XRD	ASTM D934	Identification of crystalline phases and structure
FTIR	ASTM E1252	Analysis of chemical bonding and functional groups

Table 5. Thermal stability analysis of polymer composite materials using TGA.

Sample ID	Polymer Matrix	Reinforcement Filler	Initial Decomposition Temperature (°C)	Maximum Degradation Temperature (°C)	Residual Weight (%)	Weight Loss (%)	Thermal Stability Improvement (%)
TGA-1	Epoxy	CNT	312	468	18.6	81.4	14.2
TGA-2	PP	Glass Fiber	298	452	15.3	84.7	10.8
TGA-3	PE	Nano Silica	305	460	17.9	82.1	12.6
TGA-4	Epoxy	GO	325	481	21.4	78.6	18.3
TGA-5	Polyester	Clay Nanoparticles	301	455	16.7	83.3	11.5
TGA-6	PA	Carbon Fiber	318	474	19.8	80.2	15.7
TGA-7	Vinyl Ester	Aluminum Oxide	296	448	14.9	85.1	9.6
TGA-8	Epoxy	Hybrid CNT/SiO_2	334	492	23.6	76.4	20.4

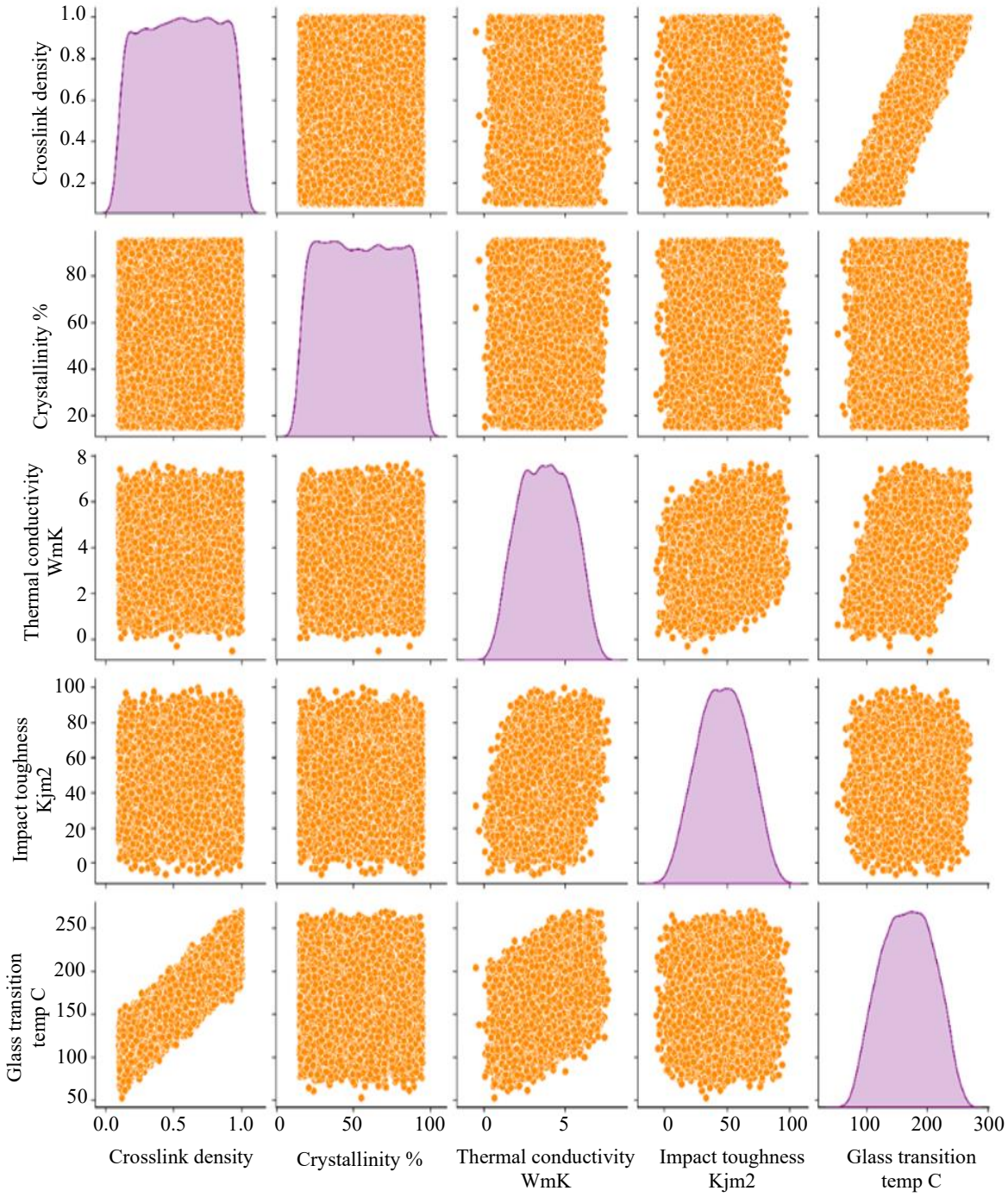

Figure 2. Correlation analysis of polymer composite material properties.

Young's modulus and tensile strength values for various composite samples are plotted in comparison in Figure 4(a). Figure 4(b) Impact toughness distribution analysis illustrating variation in energy absorption capability among the fabricated composites. Figure 4(c) RL optimization curve showing reward score variation during iterative DQN-based composite material optimization.

Comparative Analysis

In this section, a comparison of the proposed RL model based on the DQN algorithm is made with other models, such as RNN, RNN-LV, DT, and RF, using MSE and MAE measures in order to predict properties of PC. It is seen that the DQN model performs better than others.

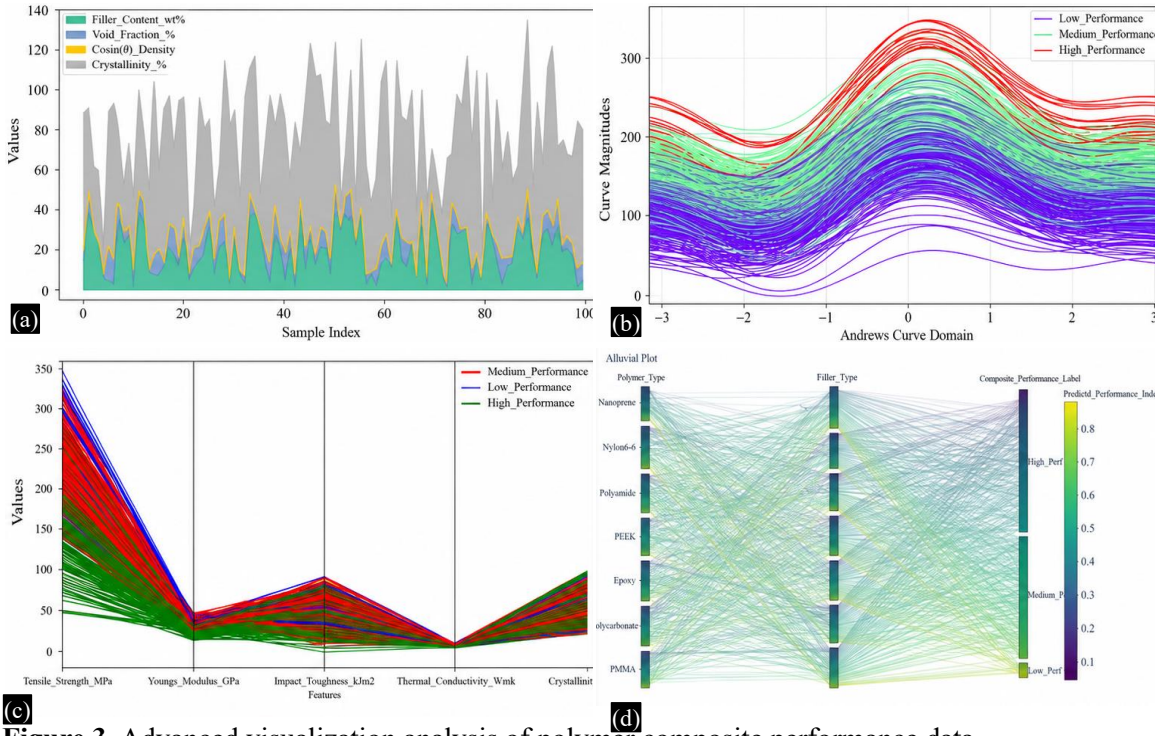

Figure 3. Advanced visualization analysis of polymer composite performance data.

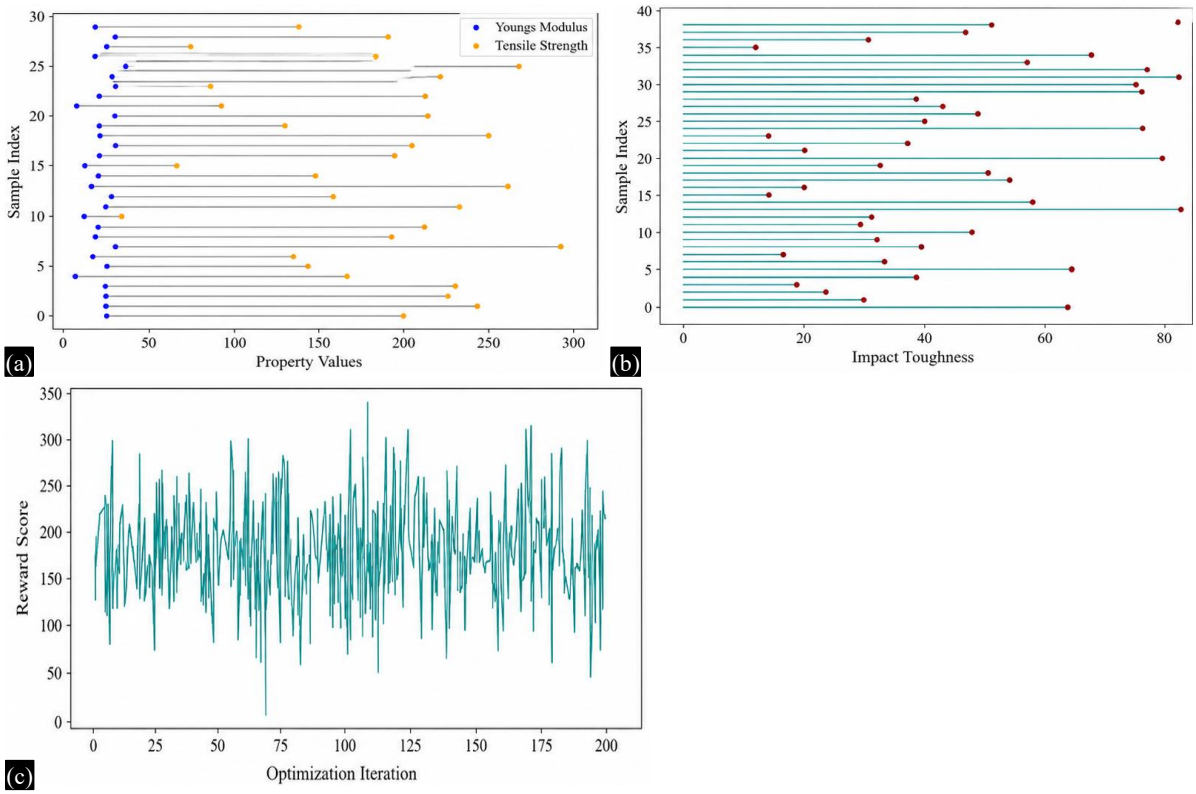

Figure 4. Mechanical property and RL optimization analysis.

The accuracy with which the suggested RL model based on DQN predicted the parameters of the polymer composite material was assessed using Mean Squared Error (MSE). Elongation, impact strength, Young's modulus, and Tensile strength, were among the mechanical parameters of the material for which the MSE calculated the deviation of squares between the experimental and anticipated values.

It was shown that the proposed model is a good representation of the nonlinear nature of the structural properties of the composites, since the MSE scores were relatively low. The mean absolute deviation of the predicted performance measures of the composites was calculated by the Mean Absolute Error (MAE). The difference between the obtained performance metrics of the composites and experimental data was measured using MAE. The proposed approach proved its effectiveness since the prediction error decreased as the MAE decreased. The suggested DQN model was trained using a dataset of WS2 nanosheet composites, sepiolite fillers, and Poly (3-hydroxybutyrate) (P3HB) reinforced with multiwalled carbon nanotubes (MWCNTs) [19].

The database included information on material parameters, filler quality, and mechanical performance factors. Comparisons with existing models were done by experimental results, which demonstrated that the proposed DQN model is better than the existing models, such as RNN-Levenberg's algorithm (LV) [19], Decision Tree (DT) [19], Recurrent Neural Network (RNN) [19], and RF [19], shown in Table 6. In the prediction of the polymer composite's Properties, the DQN framework effectively improved performance in terms of the MSE and MAE values while effectively optimizing the structure–property relationships.

The proposed DQN model and existing RNN [19], RNN-LV [19], DT [19], and RF [19] were trained on the Polymer Composite Properties Dataset, consisting of 12,700 records of polymer matrices, reinforcement fillers, processing conditions, thermal behavior, and mechanical properties. In comparison to the other models, such as RNN [19], RNN-LV [19], DT [19], and RF [19], the experimental findings showed that the suggested model based on DQN achieved reduced MSE and MAE values in the prediction of Properties. The model's capacity to optimize the structure-property relationships of PC in Table 7 and Figure 5 has been confirmed by the results.

Discussion

Research uses RL together with material characterization experiments for the optimization of the relationships between structure and property of PC. The structure-property relationship was assessed with the aid of techniques including SEM, XRD, FTIR, and TGA, while the mechanical properties were assessed in accordance with ASTM standards. DQN RL agent used the experimental dataset to optimize the polymer structure parameters, including chain structure, crosslinking density, and filler distribution.

The created ML [19] models were tailored to P3HB-based nanocomposites reinforced by WS_2 nanosheets, MWCNTs, and SEP nanoclay, thus limiting the application potential to other polymer materials. The number of samples used and the types of fillers considered were small, which might have

Table 6. Performance comparison of existing models and proposed DQN-based RL agent for polymer composite property prediction.

Metrics	RNN-LV [19]	DT [19]	RNN [19]	RF [19]	DQN [Proposed]
Elongation at break					
MAE	0.3307	0.4667	0.3095	0.5690	0.2841
MSE	0.1433	0.3020	0.1295	0.3942	0.1016
Impact strength					
MAE	2.8248	3.6911	1.9010	3.4261	1.7423
MSE	11.3285	17.0465	5.5034	16.2880	4.1027
Tensile strength					
MAE	0.5517	0.7800	0.544431	0.6860	0.5218
MSE	0.3932	0.9812	0.435228	0.6429	0.3745
Young's modulus					
MAE	0.2517	0.5822	0.2340	0.7652	0.2173
MSE	0.0806	0.4170	0.1212	0.6560	0.0621

impacted the ability of the models to generalize well and led to the risk of overfitting. Another drawback of this research was that only the mechanical properties were examined, although some other parameters, like thermal conductivity, electrical conductivity, and durability properties, could be considered.

The research aims to overcome some shortcomings of previous studies by employing a larger and more varied dataset comprising 12,700 samples, thus enhancing the model's ability to generalize. This research incorporates mechanical and thermal properties together with SEM, XRD, FTIR, and TGA examinations to allow for a more thorough analysis of the relationship between the structure and the properties of the polymers.

Table 7. Prediction performance comparison of polymer composite models.

Metrics	RNN-LV	DT	RNN	RF	DQN
Elongation at break					
MAE	0.3140	0.4413	0.2753	0.5320	0.2694
MSE	0.1358	0.2870	0.1077	0.3722	0.0857
Impact strength					
MAE	1.5708	2.1077	1.7580	1.3984	1.5607
MSE	10.5603	15.7895	4.7841	14.0871	3.5042
Tensile strength					
MAE	0.5368	0.7620	0.525788	0.6610	0.5017
MSE	0.3744	0.9514	0.415670	0.6377	0.3520
Young's modulus					
MAE	0.2380	0.5675	0.2166	0.7413	0.1850
MSE	0.0635	0.3850	0.1047	0.5823	0.0478

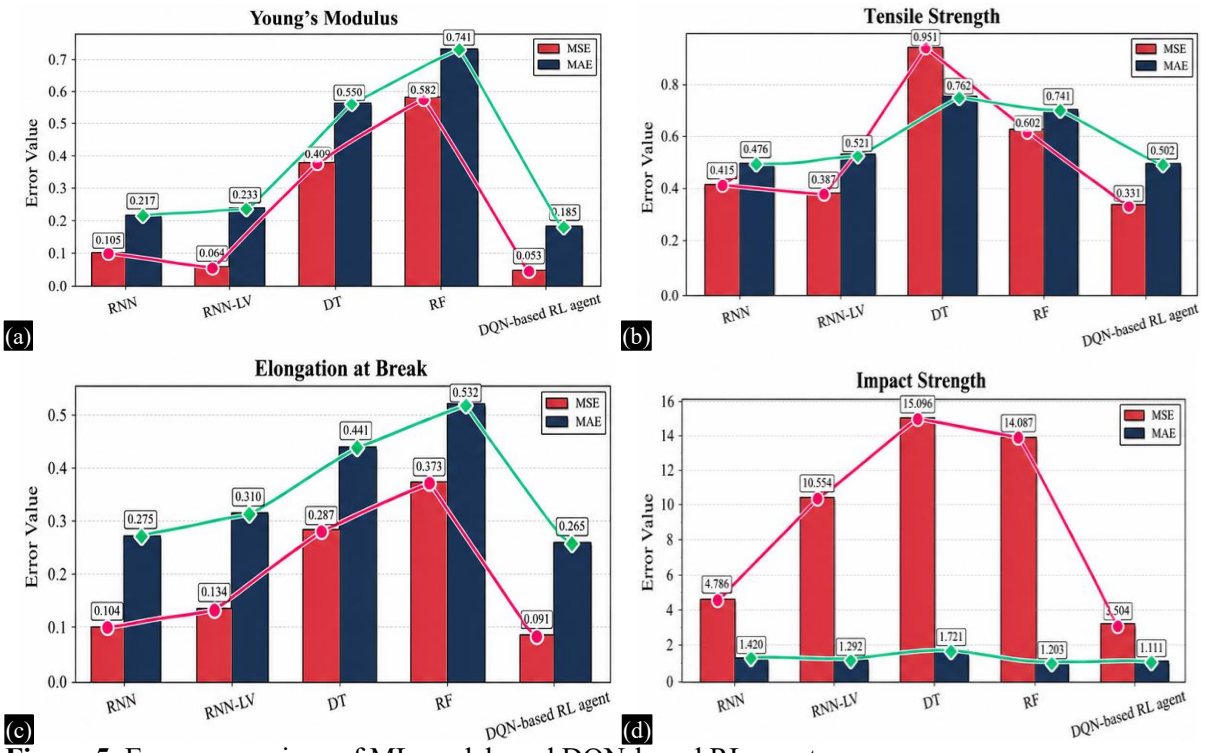

Figure 5. Error comparison of ML models and DQN-based RL agent.

CONCLUSION

The optimization of the relation between the structure and properties of PC is considered to be a very complex task because of the complicated nonlinear interrelation between the materials used and the parameters of their processing. Optimization requires much time, which makes traditional approaches ineffective. To optimize the parameters, the RL system based on DQN with the help of SEM, XRD, FTIR, TGA, and ASTM tests was built on the basis of the Polymer Composite Properties Dataset including 12,700 samples. The findings demonstrate that the algorithm provided the lowest prediction error for the properties, with MSE values of 0.0478, 0.3520, 0.0857, and 3.5042, respectively, and MAE values of 0.1850, 0.5017, 0.2694, and 1.5607, respectively. It should be noted, however, that the research was limited to a few types of polymers and laboratory testing, while electrical conductivity and durability were not studied sufficiently.

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