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Artificial Intelligence and Machine Learning for Composite Materials Design

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Artificial Intelligence and Machine Learning for Composite Materials Design

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Artificial intelligence is becoming a powerful tool to design and develop new materials, especially in composite materials design. Fiber-reinforced polymer composites have an exceptional advantage over traditional materials for their superior or specific stiffness and strength, and resistance to corrosion and fatigue, which results in low total lifetime cost. One of the primary limitations of these composite materials is predicting mechanical, thermal, and electrical properties due to the anisotropy of the materials. Predicting mechanical, thermal, and electrical properties is important in utilizing these composite materials for multiple engineering applications. To address this issue requires a machine learning model trained from large composite materials structure property and performance relationship. In recent years artificial intelligence and machine learning have shown substantial interest in predicting different properties of composite materials. More exploration needs to be required to predict the mechanical, thermal, and electrical properties of composite materials using artificial intelligence and machine learning. Firstly, this research aims to review and understand data-driven computational methods to design and analyze fiber-reinforced composite materials. Secondly, to develop an experimental database of reinforced composite materials. Finally, to design and develop artificial intelligence and machine learning courses for undergraduate mechanical engineering technology students.

Keywords: Machine Learning, Property Prediction, Composite Materials

Introduction

Modern engineering applications focus on designing novel materials with superior tailored properties, leveraging advancements in high-performance parallel computing, materials science, and numerical modeling. These advancements allow for the calculation of many essential properties of materials, marking a significant shift in material science and engineering [1]. Material design comprises forward modeling problems, where the structure of a material is given and its properties are determined by physical laws, and inverse design problems, where the goal is to generate a material structure with a set of required properties. While physics-based modeling tools can address forward problems, inverse design problems often rely on domain knowledge, experience, and trial-and-error approaches. Machine learning is a branch of artificial intelligence, using statistical and probabilistic methods to learn from experience and detect hidden patterns in data. Machine learning algorithms can detect patterns and learn a function that best maps input variables to output variables, a procedure referred to as the training process. This capability can significantly accelerate the discovery and design of materials. A significant portion of Machine learning applications in materials science focus on discovering new chemical compounds or molecules with desired properties, a subfield known as Machine Learning for materials chemistry. Feature engineering, the process of finding a suitable representation of a molecule or crystal structure for Machine Learning models, is a critical aspect of this subfield. Comprehensive materials databases, like the Materials Project and Open Quantum Materials Database, provide access to abundant data, facilitating the discovery of new compounds. Composite materials, composed of two or more base materials, offer a vast design space and unique properties. Recent advances in additive manufacturing have expanded the possibilities for creating complex materials with internal voids and multiple materials.

Material science has shifted from purely computational techniques to coupled methods integrating computational predictions with experimental validation. Machine Learning offers a broader scope for studying composites' behavior, allowing for simultaneous exploration of multifunctional properties. Despite the constraints posed by multiple variables, Machine Learning has proven effective in addressing increased dimensionality and uncertainty in data [2]. Although there are significant advancements in Machine Learning, there are challenges in understanding the relationship between input design parameters and output strength of the reinforced composite. However, these machine learning models cannot provide the required support to design reinforced composite materials. Mostafa et al. [3] introduces an explainable Artificial Intelligence (XAI) framework that will help to understand the input–output relationships of the machine learning model using SHapley Additive exPlanations (SHAP) and Partial Dependence Plots (PDPs). At the same time, this model provides for a design approach for making adjustment of the important parameters to get the desired reinforced composite strength by using an explainability technique known as Counterfactual (CF). This framework can help designers understand input parameters and their relationship with the desired strength of materials. This model will also allow the designer to control corresponding design parameters to get the desired strength of the reinforced composites. Vahid et al. [4] discussed explainable artificial intelligence techniques to predict defect characterization in reinforced composite materials. They developed explainable decision tree-based machine learning models with transparent decision paths-based features to predict the defect depth, thickness and size.

In this research, the first aim is to review and understand data-driven computational methods to design and analyze fiber-reinforced composite materials. Secondly, to develop an experimental database of reinforced composite materials. Finally, to design and develop artificial intelligence and machine learning courses for undergraduate mechanical engineering technology students.

1. **Review and understand data-driven computational methods to design and analyze fiber-reinforced composite materials**

Machine Learning Models

To use artificial intelligence for design reinforced composite materials, it is important to understand the terms artificial intelligence and machine learning. Artificial intelligence is the process of exhibiting human intelligence by machine. Whereas machine learning is a method of achieving artificial intelligence. There are several approaches used to classified machine learning models such as i) supervised learning ii) unsupervised learning and iii) reinforcement learning [5]. Supervised machine learning is used for making predictions from known sets of data or sometimes known as ground truth. In this method it is important to know the target variables or what needs to be predicted. The known datasets are used to train the machine learning algorithms which can predict the output. On the other hand, unsupervised learning is helpful where the target variables are unknown. Unsupervised machine learning are data-driven methods that trained with unlabeled data to search for undetected patterns of the variables. Reinforcement machine learning is different from supervised learning and unsupervised learning. In reinforcement learning does not require labeled data or a training set. It depends on the ability to measure the response to the actions of the learning tool. In reinforcement learning method, learning algorithms train in an environment by itself. Machine learning is one of the most powerful artificial intelligence technologies which can help to composite materials design. Gelayol et al. [6] performed a study to explore the use of Machine Learning in predicting mechanical properties of carbon fibers with limited data. Employing a Taguchi Design of Experiments (DOE) approach, combined with Support Vector Regression (SVR) and Artificial Neural Network (ANN), the research aims to develop robust prediction tools using empirical models. These models are based on three parameters from the stabilization process of oxidized Polyacrylonitrile (PAN) fibers. The study reveals that SVR models perform better in predicting Young's modulus, while ANN models excel in predicting tensile strength, demonstrating ML's potential in high-tech manufacturing with limited datasets.

Challenges and Applications of Artificial Intelligence on Composite Material Design

However, machine learning has huge potential to be successful at the same time needs to address some drawbacks, challenges, and limitations. Onyeka et al. [7] summarizes challenges and opportunities of artificial intelligence on composite material design. Several factors may affect output of reinforced composites materials design such as reliable sources of input data, physic-chemical reaction of polymer [8]. Material design comprises forward modeling problems, where the structure of a material is given and its properties are determined by physical laws, and inverse design problems, where the goal is to generate a material structure with a set of required properties. While physics-based modeling tools can address forward problems, inverse design problems often rely on domain knowledge, experience, and trial-and-error approaches. In this project the objective is to use artificial intelligence and machine learning for composite materials design. To overcome potential challenges, an experimental database for reinforced composite materials was developed.

2. Development of Mechanical Database Reinforced Composite Materials

For the development of the experimental database chopped fiber reinforced composite panels were fabricated and performed mechanical tests such as flexure and compression test.

Table 1: Flexure Test Results (Glass Fiber Percentage Study)

Fiber %	SP #	Strength at Fracture, σ_f, psi			Modulus, ksi		
			Average	STD		Average	STD
1 %	1	2,885	2,564	241	665	683	16
	2	2,504			680		
	3	2,303			705		
2 %	1	2,554	2,618	59	610	603	5
	2	2,697			600		
	3	2,604			600		
3 %	1	4,554	4,643	147	800	833	40
	2	4,850			890		
	3	4,525			810		
4 %	1	2,982	2,875	96	640	638	2
	2	2,750			635		
	3	2,892			640		

Flexure Test of Reinforced-Composite

A flexible test was performed using MTS machine (ASTM D 790). The displacement rate was 0.1 in/min and 400 lb. load cell was used to apply the load and 2 data was collected every second. Machine displacement was considered as specimen deformation to calculate flexural modulus. The load was applied in thickness direction of the panel. Table 1 shows the flexure test results of glass fiber reinforced composite at different percentages of fiber loading. Table 2 shows the flexure test results of glass fiber reinforced composite at different length and diameter of reinforced fiber.

Table 2: Flexure Test Results (Glass Fiber Length and Diameter Study)

Panel #	Fiber	Density, g/cc	SP #	Flexure Strength, psi	Av.	STD.	Flexure Modulus, ksi	Av.	STD.
Panel #1	Type I (1/2in)	1.03	1	2,801	2,801	81	503	503	2.9
			2	2,900			500		
			3	2,702			507		
Panel #2	Type I (1/4in)	1.06	1	2,922	2,880	192	500	484	11.7
			2	2,627			472		
			3	3,091			481		
Panel #3	Type I (1/6in)	1.05	1	3,121	3,096	134	506	506	1.2
			2	3,247			507		
			3	2,921			504		
Panel #4	Type II(1/4in)	1.09	1	3,700	3,667	90	594	593	8.6
			2	3,756			603		
			3	3,544			582		
Panel #5	Type II (1/2in)	1.11	1	3,100	3,269	190	612	599	12.0
			2	3,172			583		
			3	3,535			602		
Panel #6	No Fiber	1.04	1	2,316	2,360	72	520	507	16.1
			2	2,462			516		
			3	2,303			484		

Table 3: Compression Test Results (Glass Fiber Percentage Study)

Fiber %	SP #	Density, g/cm3	Max Strength σ_{cult}, or Strength at 5% strain $\sigma_{5\%}$, psi			Modulus, ksi		
				Average	STD		Average	STD
1%	1	1.14	4,678	3,612	750	321	191	78
	2		4,302			240		
	3		3,271			145		
	4		3,111			131		
	5		2,699			119		
2%	1	1.10	3,961	3,402	297	163	143	13
	2		3,324			146		
	3		3,312			131		
	4		3,349			148		
	5		3,066			125		
3%	1	1.29	5,735	4,437	1,127	200	170	20
	2		5,175			174		
	3		5,107			180		
	4		2,987			149		
	5		3,182			148		
4%	1	1.10	3,199	3,231	83	116	135	12
	2		3,302			135		
	3		3,198			143		
	4		3,346			129		
	5		3,111			150		

Compression Test

Compression test was performed to measure compression strength and modulus of reinforced composites using MTS machine (ASTM D 695). The displacement rate was 0.05 in/min and 1,000 lb. load cell was used to apply the load and 1 data was collected every second.

Machine displacement was considered as specimen deformation to calculate modulus. Table 3 summarizes all compression test results of glass fiber reinforced composite at different percentages of fiber loading.

3. Course Development of Undergraduate Mechanical Technology Students

The mechanical engineering industry is expecting significant changes toward machine learning and artificial intelligence. To adapt to this new technology, it is important to design and develop new courses to fit the students of mechanical engineering technology.

Syllabus

MTC 4XX: Machine Learning to Composite Material Design
SUNY Polytechnic Institute
Department of Engineering Technology
Online

Course Description:

This course is designed for undergraduate mechanical engineering technology students with fundamental knowledge in programming and machine learning, artificial intelligence aiming to apply these tools to design composite materials. This course also introduces the concept of fiber reinforced composite materials, anisotropic theory, constitutional equations, stress analysis, and test methods for composites. Students will understand the design of a general class of large and complex composite structures.

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Course Schedule and Topics:

Module 1 (Week 1-2)

- ✓ Review Statics and Strength of Materials
- ✓ Materials, Stress and Deformation Analysis
- ✓ Design for Different Types of Loading
- ✓ Failures Resulting from Static Loading
- ✓ Fatigue Failure Criteria for Fluctuating Stress

Module 2 (Week 3-4)

- ✓ The concept of fiber reinforced composite materials, anisotropic theory, constitutional equations, stress analysis, and test methods for composites
- ✓ Classification of anisotropy and associated elastic constants, micromechanics models, theory of failures, classical laminate theory of bending, special types of laminates, hygrothermal effects, and test methods
- ✓ Modeling, stress and deflection analysis of fiber reinforced composites using computational tool
- ✓ Application of composite materials to the design and analysis of structures.

Module 3 (Week 5-10)

- ✓ Machine Learning Fundamentals
- ✓ Popular Supervised Machine Learning Techniques
- ✓ Unsupervised Machine Learning Techniques
- ✓ Describe the basic concepts of optimization, Machine Learning (ML)

Module 4 (Week 11-15)

- ✓ Introduction to Python
- ✓ Develop Python 3+ programming scripts to implement several ML
- ✓ Material property prediction
- ✓ Design optimization using machine learning

Conclusion:

In recent years artificial intelligence and machine learning have shown substantial interest in predicting different properties of composite materials. Although there are significant advancements in Machine Learning, there are challenges in understanding the relationship between input design parameters and output strength of the reinforced composite. More exploration needs to be required to predict the mechanical, thermal, and electrical properties of composite materials using artificial intelligence and machine learning. Machine Learning algorithms will be developed and will be compared with experimental data. The mechanical engineering industry is expecting significant changes toward machine learning and artificial intelligence. To adapt to this new technology, it is important to design and develop new courses to fit the students of mechanical engineering technology.

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