

MACHINE-LEARNING-ASSISTED DESIGN OF COMPOSITE MATERIALS

A THESIS

submitted by

PRIYA NAIR

for the award of the degree

of

DOCTOR OF PHILOSOPHY

DEPARTMENT OF METALLURGICAL AND MATERIALS ENGINEERING
NATIONAL INSTITUTE OF TECHNOLOGY
TIRUCHIRAPPALLI - 620015

MAY 2026

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THESIS CERTIFICATE

This is to certify that the thesis entitled **Machine-Learning-Assisted Design of Composite Materials** submitted by Priya Nair to the National Institute of Technology, Tiruchirappalli for the award of the degree of Doctor of Philosophy is a bonafide record of research work carried out under my supervision. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

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Date:

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Guide

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ABSTRACT

Fibre-reinforced polymer composites are designed by choosing fibres, matrix, layup and processing conditions, and each candidate is traditionally tested by expensive experiments or finite-element simulation. This thesis builds machine-learning surrogates that predict the stiffness and strength of laminated composites from their design variables, and uses them to search the design space. A Gaussian-process surrogate trained on 600 finite-element simulations predicts laminate stiffness within 3% and guides a Bayesian optimization that finds layups 18% lighter than a baseline design at equal stiffness, confirmed by three physical tests.

Keywords: composite materials, machine learning, Gaussian processes, Bayesian optimization, laminate design

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Chapter 1

INTRODUCTION

Composite laminates let engineers tailor stiffness and strength to the loads a part will carry, but the design space is vast: fibre type, matrix, ply angles, ply count and cure cycle all matter. Physical testing is slow and simulation is costly. Machine-learning surrogates can approximate the simulation at a fraction of its cost and make systematic search possible.

Chapter 2

BACKGROUND

Classical lamination theory relates in-plane forces N and moments M to mid-plane strains ε^0 and curvatures κ through the stiffness matrices A , B and D ,

$$\begin{bmatrix} N \\ M \end{bmatrix} = \begin{bmatrix} A & B \\ B & D \end{bmatrix} \begin{bmatrix} \varepsilon^0 \\ \kappa \end{bmatrix}. \quad (2.1)$$

Gaussian processes model an unknown function with a prior over functions and give calibrated uncertainty [2], which Bayesian optimization uses to choose the next design to evaluate [1].

Chapter 3

SURROGATE MODELLING AND OPTIMIZATION

We parameterize a laminate by its ply angles and fibre volume fraction, train a Gaussian process on finite-element results, and use expected improvement to propose layups that minimize mass at a required stiffness.



Figure 3.1: Surrogate-assisted design loop.

Chapter 4

RESULTS AND DISCUSSION

Table 4.1 compares the baseline and optimized layups.

Table 4.1: Baseline and optimized laminates at equal axial stiffness.

Design	Plies	Mass (g)	Measured stiffness (GPa)
Baseline quasi-isotropic	16	412	48.6
Optimized	13	338	48.9

Chapter 5

CONCLUSIONS

Surrogate models make it practical to search laminate designs that would be too expensive to explore by simulation alone. Extending the surrogate to damage tolerance and fatigue is future work.

Appendix A

FINITE-ELEMENT MODEL DETAILS

Laminates were modelled with four-node shell elements and a mesh size of 2 mm, verified by a convergence study to change the predicted stiffness by less than 0.5%.

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- [1] Donald R. Jones, Matthias Schonlau, and William J. Welch. Efficient global optimization of expensive black-box functions. *Journal of Global Optimization*, 13: 455–492, 1998.
- [2] Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian Processes for Machine Learning*. MIT Press, 2006.

LIST OF PAPERS BASED ON THESIS

1. P. Nair and S. Ramanathan, “Gaussian-process surrogates for laminate stiffness,” *Journal of Composite Design*, vol. 12, pp. 45–58, 2025.
2. P. Nair and S. Ramanathan, “Bayesian layup optimization under strength constraints,” in *Proc. National Conference on Advanced Materials*, 2025, pp. 112–118.

CURRICULUM VITAE

Priya Nair received her B.Tech. in Mechanical Engineering and her M.Tech. in Materials Engineering, and joined the Department of Metallurgical and Materials Engineering as a research scholar in 2021.

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