“Integrated Machine Learning Approaches for Advanced Analysis of Semiconductor Materials”

Aishwarya Katkar, Mechanical Engineering

Mentor: Dr. Masoud Yekani Fard, Assistant Teaching Professor

School for Engineering of Matter, Transport and Energy

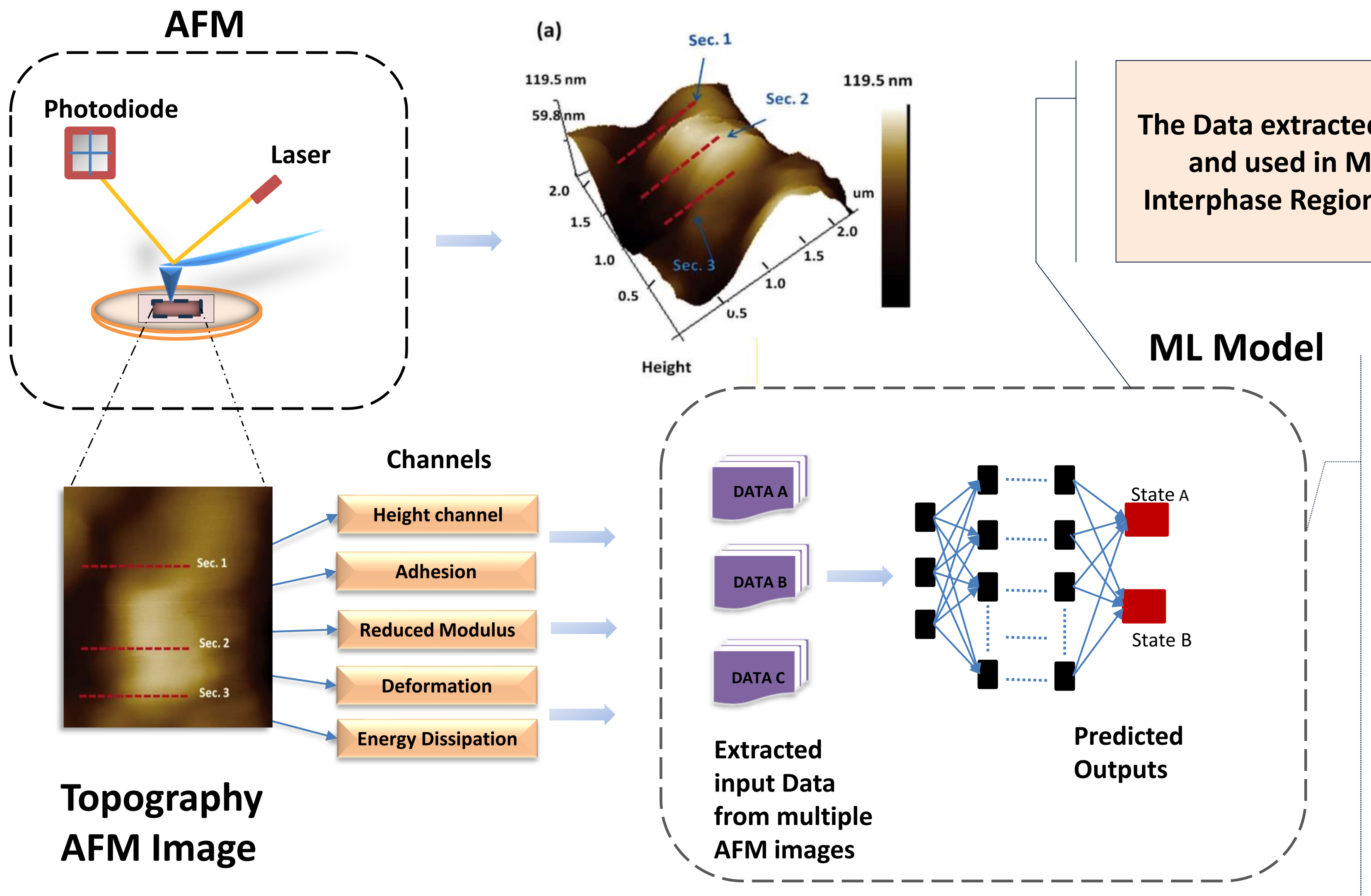
Research Motivation

- **Advancement in Semiconductor Materials**: The rapid evolution of semiconductor technology necessitates materials with enhanced mechanical properties to ensure their durability during fabrication and use.
- **Potential of Carbon Nanotubes (CNTs)**: Integrating CNTs into semiconductor materials has emerged as a promising approach to improve mechanical integrity, reducing the risk of failure from stresses encountered during device fabrication and operation.
- **Optimization Challenge**: Determining the optimal parameters for CNT integration (e.g., concentration, distribution, alignment) is crucial for maximizing material toughness, a process currently hindered by the time-consuming nature of empirical testing.

Goals

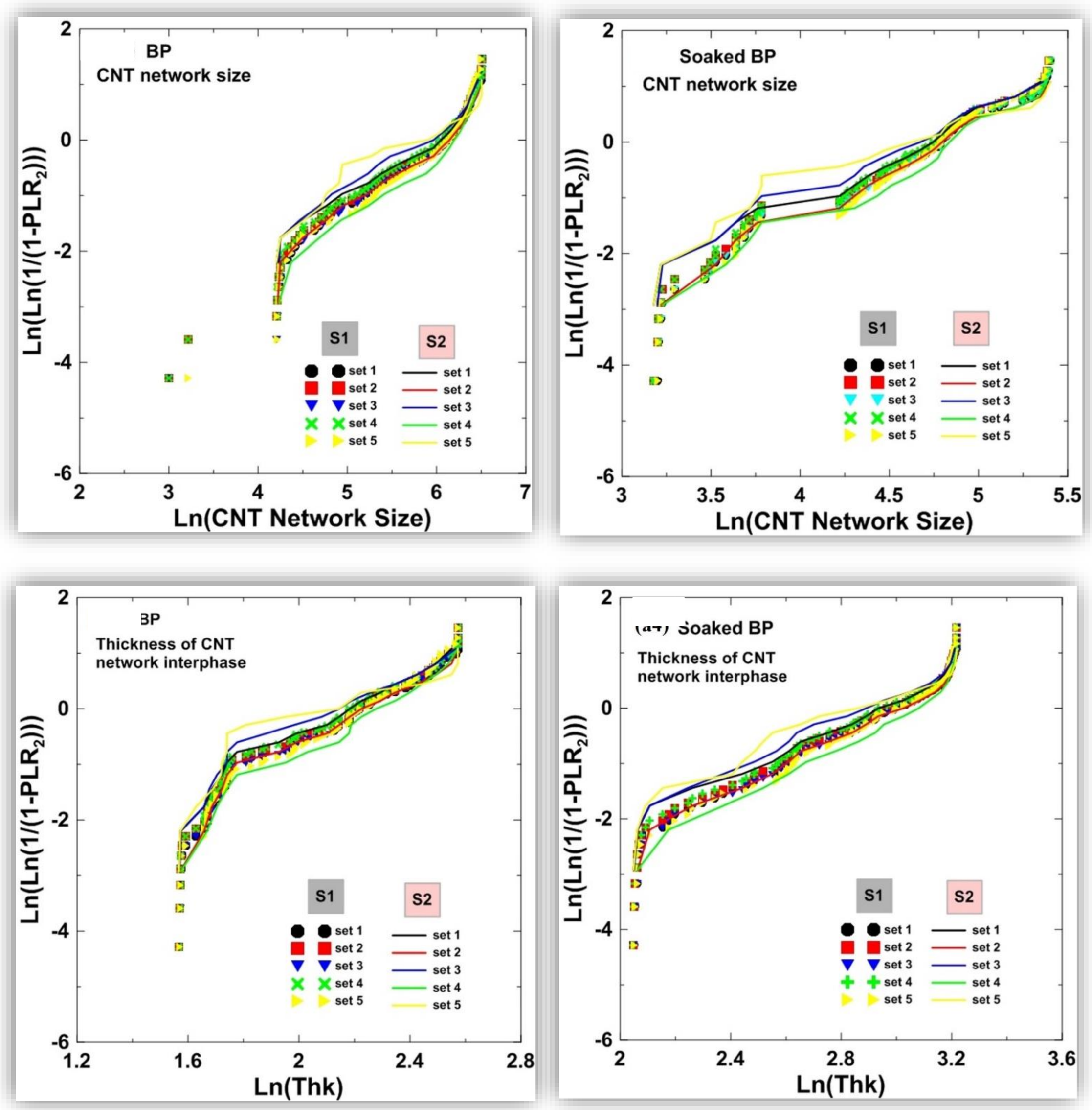
- **Machine Learning Solution**: The application of machine learning (ML) techniques offers a revolutionary pathway to efficiently predict how various CNT configurations impact material properties, overcoming the limitations of traditional testing methods.
- **Objective of Research**: To develop a predictive ML model that accurately forecasts the mechanical properties of materials based on specific CNT integration parameters, facilitating the rapid development of stronger, more resilient semiconductor materials.

Research Methodology



1.Gather and standardize data on CNT-enhanced materials.
2.Train ML models to predict material properties from CNT configurations.
3.Validate and refine model accuracy with separate datasets.
4.Deploy a prediction tool for material optimization in semiconductor manufacturing

Data Representation

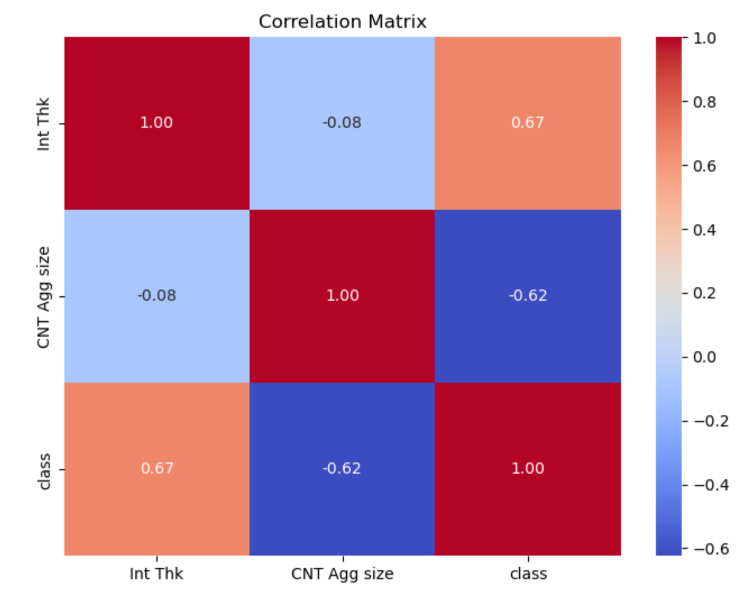


AFM Image collection: Utilizing Atomic Force Microscopy (AFM), we collect topographical images of materials under investigation.
Data Extraction: The study encompasses both dry and pre-treated bucky paper, focusing on extracting the interphase region and particle thickness from AFM data.
Machine learning Processing: The information is then processed through various machine learning models, with data segmented into training (S1) and testing (S2) subsets.
Model Challenge: The challenge lies in the overlap between data for dry and soaked Bucky paper, which complicates training the machine learning model.

Results

- It was observed that materials with larger particle sizes and smaller interphase regions exhibit enhanced properties.
- After evaluating various models, the **Random Forest** algorithm was selected for its superior performance on the test data.
- Accuracy of Model = 95.68%
- Area under the curve = 0.98

Model Evaluation



Model Report

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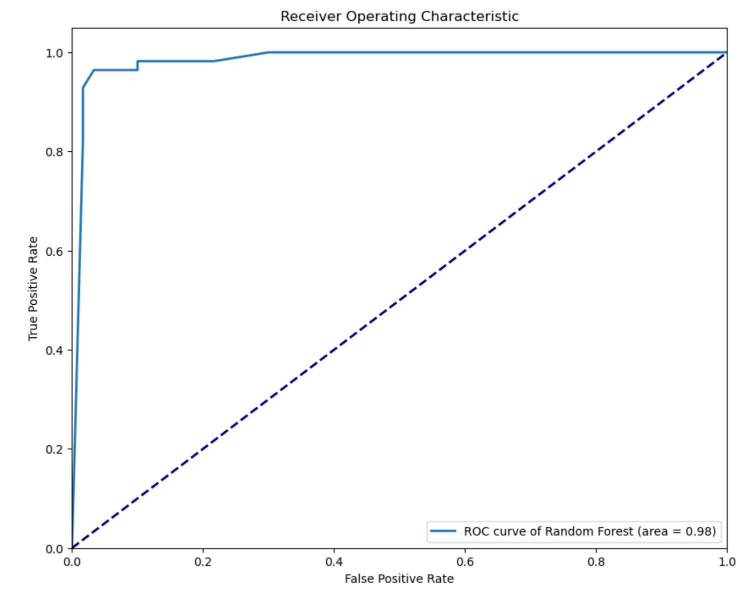
Training Random Forest...
Evaluating Random Forest...
Accuracy: 0.9568965517241379
Classification Report:
              precision    recall  f1-score   support

           0       0.94      0.98      0.96        60
           1       0.98      0.93      0.95        56

    accuracy                           0.96       116
   macro avg       0.96      0.96      0.96       116
weighted avg       0.96      0.96      0.96       116
```

ROC Curve



Future Works

Future research could focus on applying deep learning for feature extraction from AFM images across a wider array of materials and on integrating the ML model into real-world manufacturing for real-time quality control and predictive maintenance. Additionally, exploring the long-term performance and environmental sustainability of CNT-enhanced materials would be valuable.

Acknowledgement

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Fard, M. Y., Seyler, H., Tata, A., & Orozco, Y. (2023). CNT Network Size/Interphase and Multimode interlaminar fracture of CNT Buckypaper nanocomposites. *AIAA SCITECH 2023 Forum*. https://doi.org/10.2514/6.2023-1133