MSE497

Undergraduate Project

Predicting Material Properties and integrating Artificial Intelligence

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Introduction

We're building an AI/ML model to understand how different alloy compositions influence stacking fault energy (SFE) in high-strength low-alloy (HSLA) steels. SFE is a key factor affecting properties like work hardening, dislocation movement, and impact toughness, making it crucial for industries like automotive and aerospace. By leveraging machine learning, we aim to predict SFE trends based on composition, helping optimize material properties more efficiently. Our approach involves gathering data, training models to identify patterns, and using predictive analysis .

Approach to Data Collection

Literature-Based Data Collection

Research Papers & Databases
Patents & Industry Reports

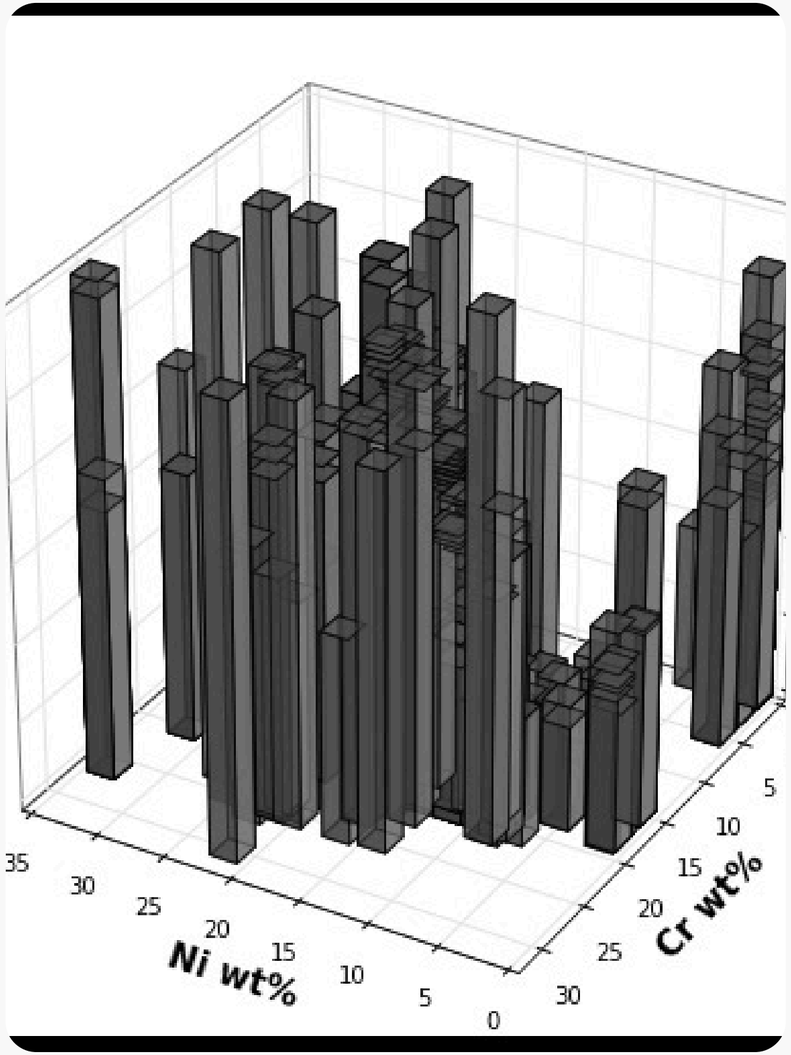
Synthetic Data Augmentation for ML Models

Predict SFE for untested compositions using probabilistic models.

Computational Data Generation

Thermo-Calc & CALPHAD Approach

Findings...

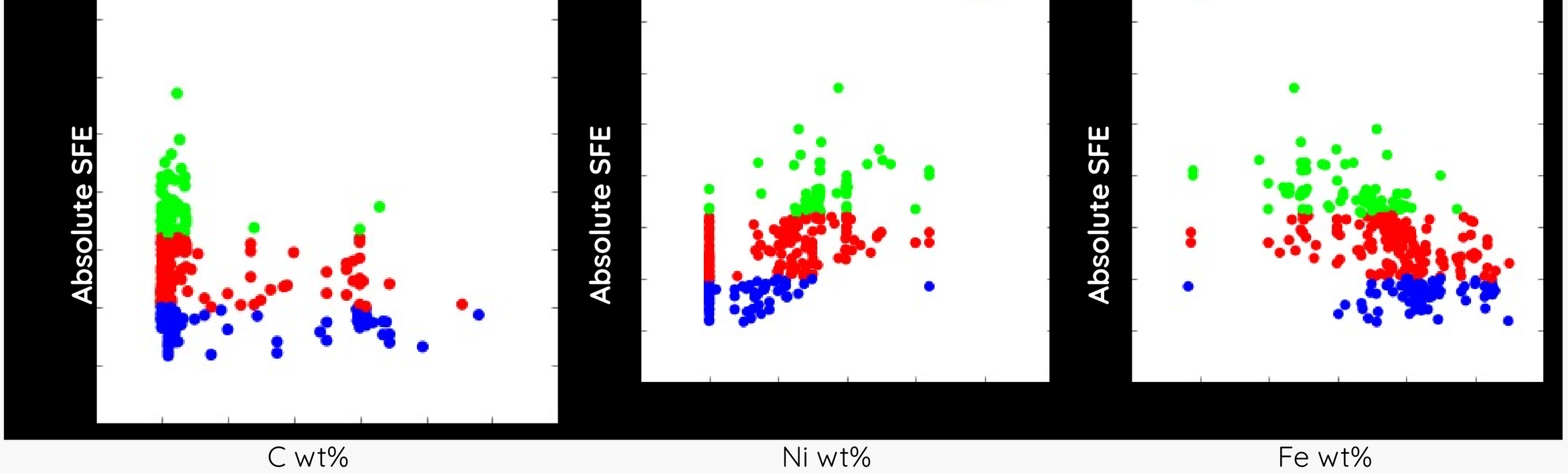


Data Collected and Reasonings -

We started off with a total of 474 data points but some did not have the Temperature readings and so refining it to 428. Them we removed the data where there was a slightest of change in the Minor elements (elements with composition <0.05)

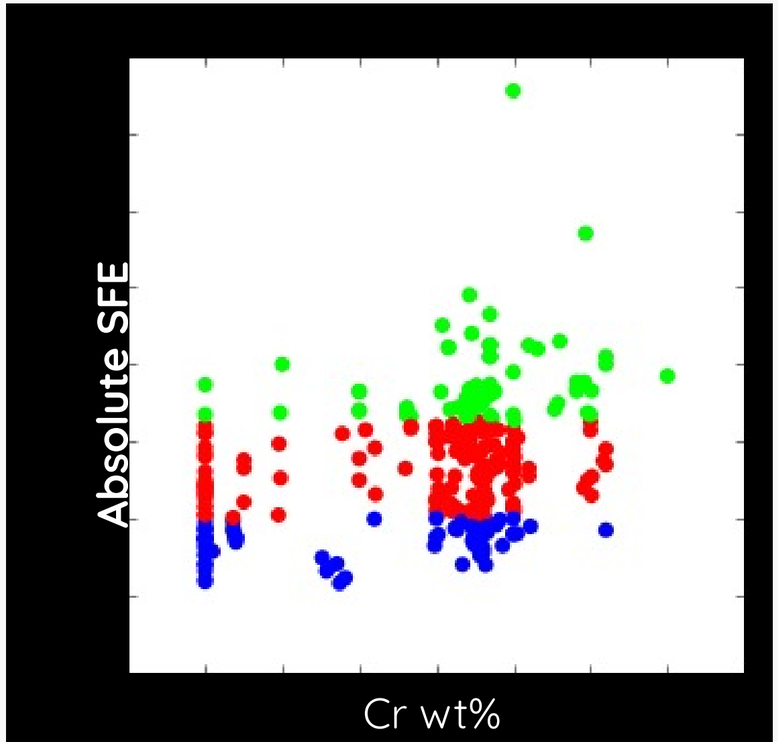
Finally we were left with 360 Data Points

For testing and selecting the model, we need an unseen test set. Hence we take our data and split it into an 80:20::train:test sets. We will build our models on the training set and then test their performance on "unseen" test set to finally select our best performing (one that generalizes well to unseen data) model.



Measurement Scales

Absolute SFE - mJ/m^2

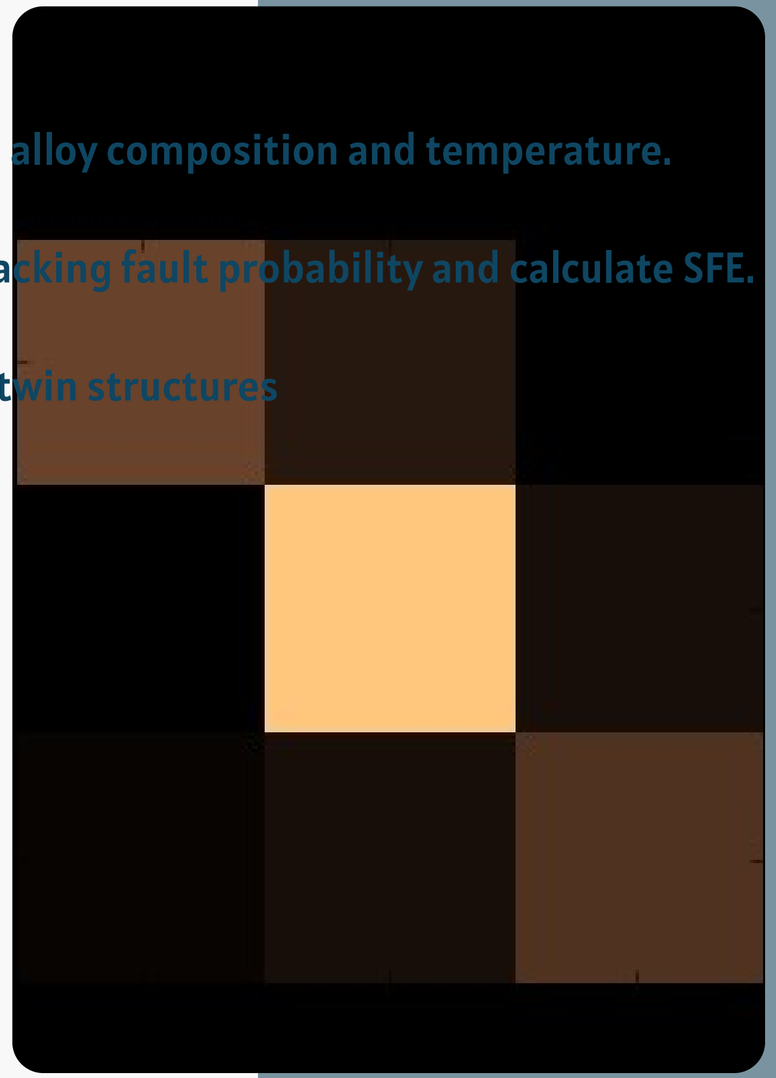


Methodology

Methods of SFE Evaluation

- Thermodynamic Models: Use equilibrium calculations to estimate SFE based on alloy composition and temperature.
- X-ray and Neutron Diffraction: Measure diffraction peak broadening to infer stacking fault probability and calculate SFE.
- Transmission Electron Microscopy (TEM): Directly observes stacking faults and twin structures
- Prediction Models Used -

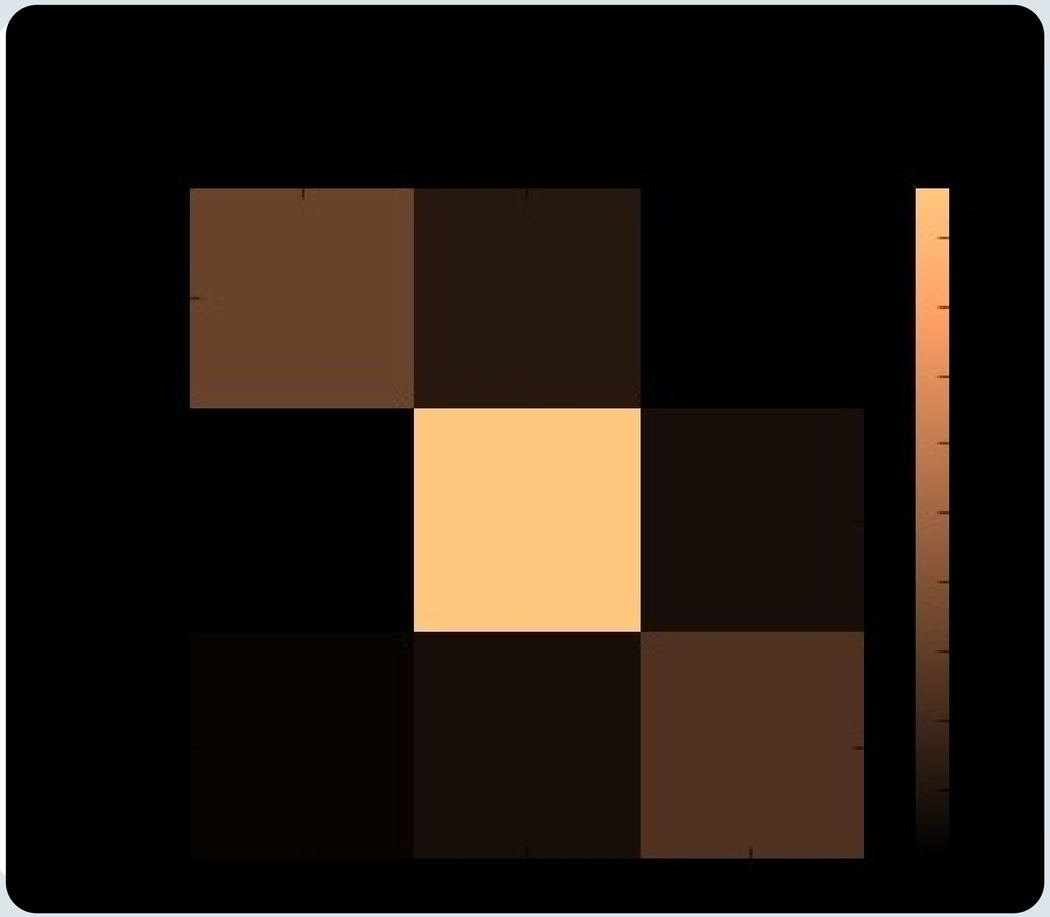
1. SVM (Support Vector Machine)
2. Random Forest Model



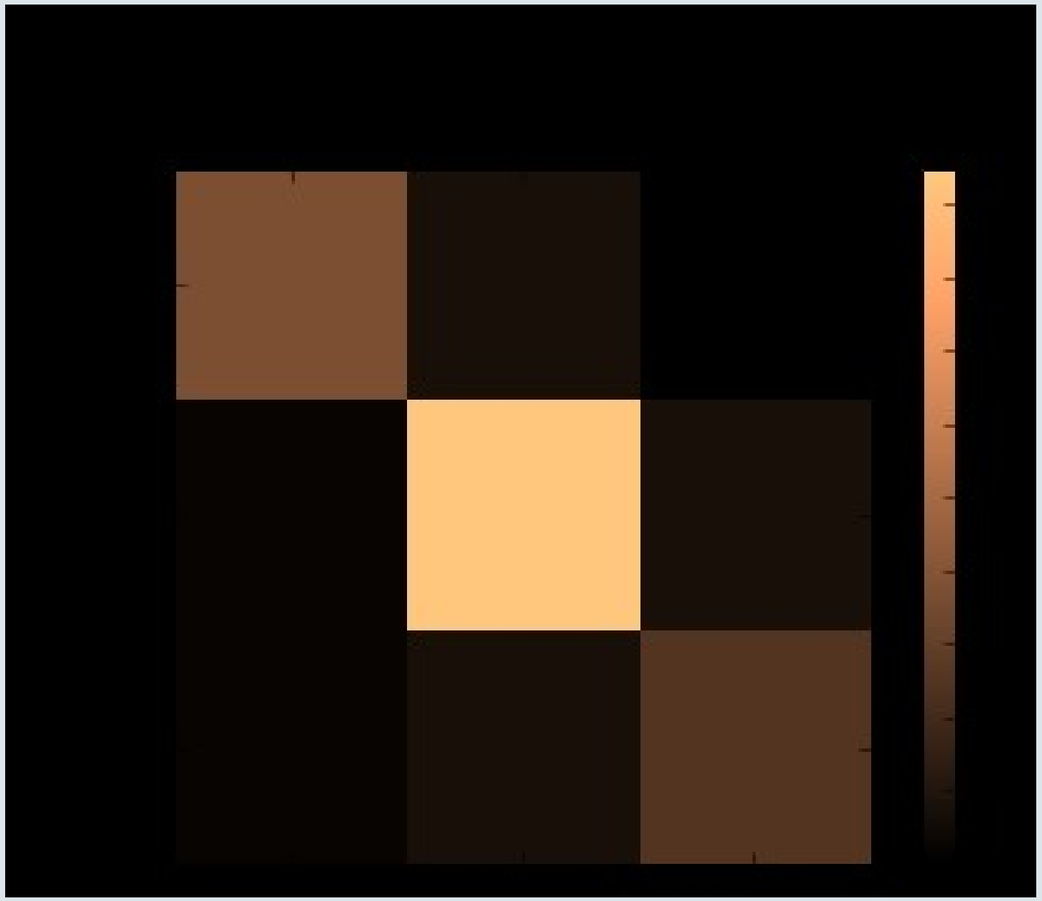
Data Analysis -

Model scores are technical measures of how well your models are able to predict the training data

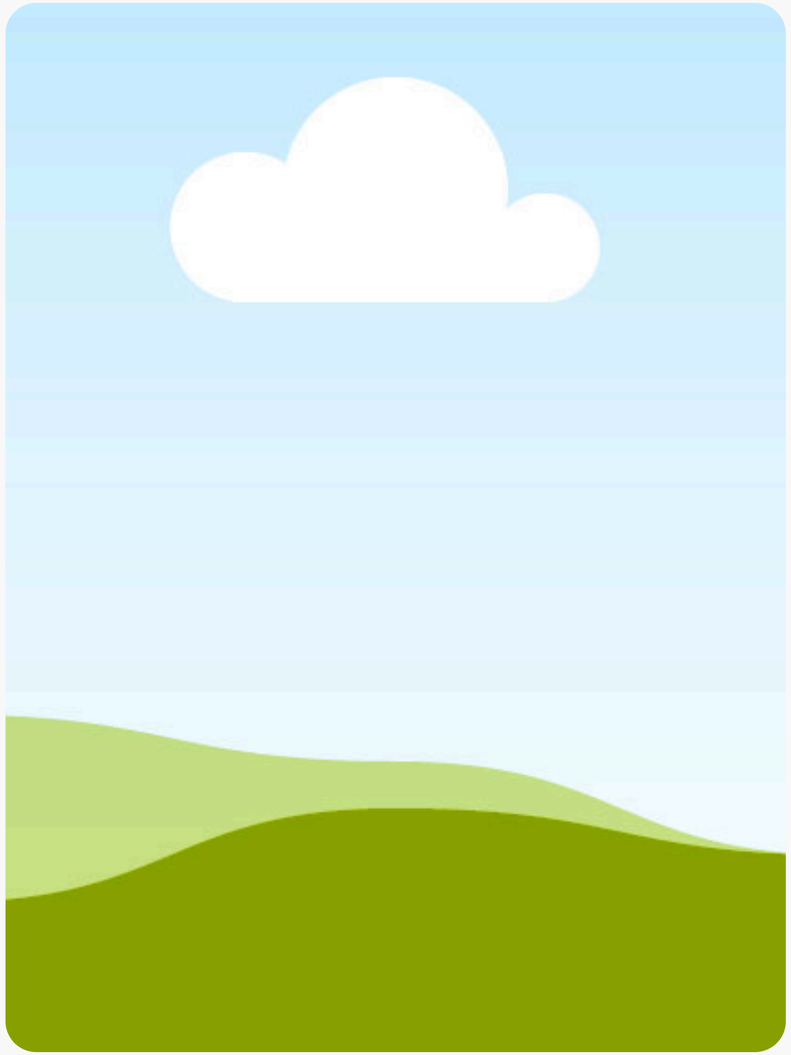
Model Score for SVM on actual Data 0.84
Model Score for SVM on training Data 0.87



Model Score for RF on actual Data 0.85
Model Score for RF on training Data 0.99



Random Forest Model

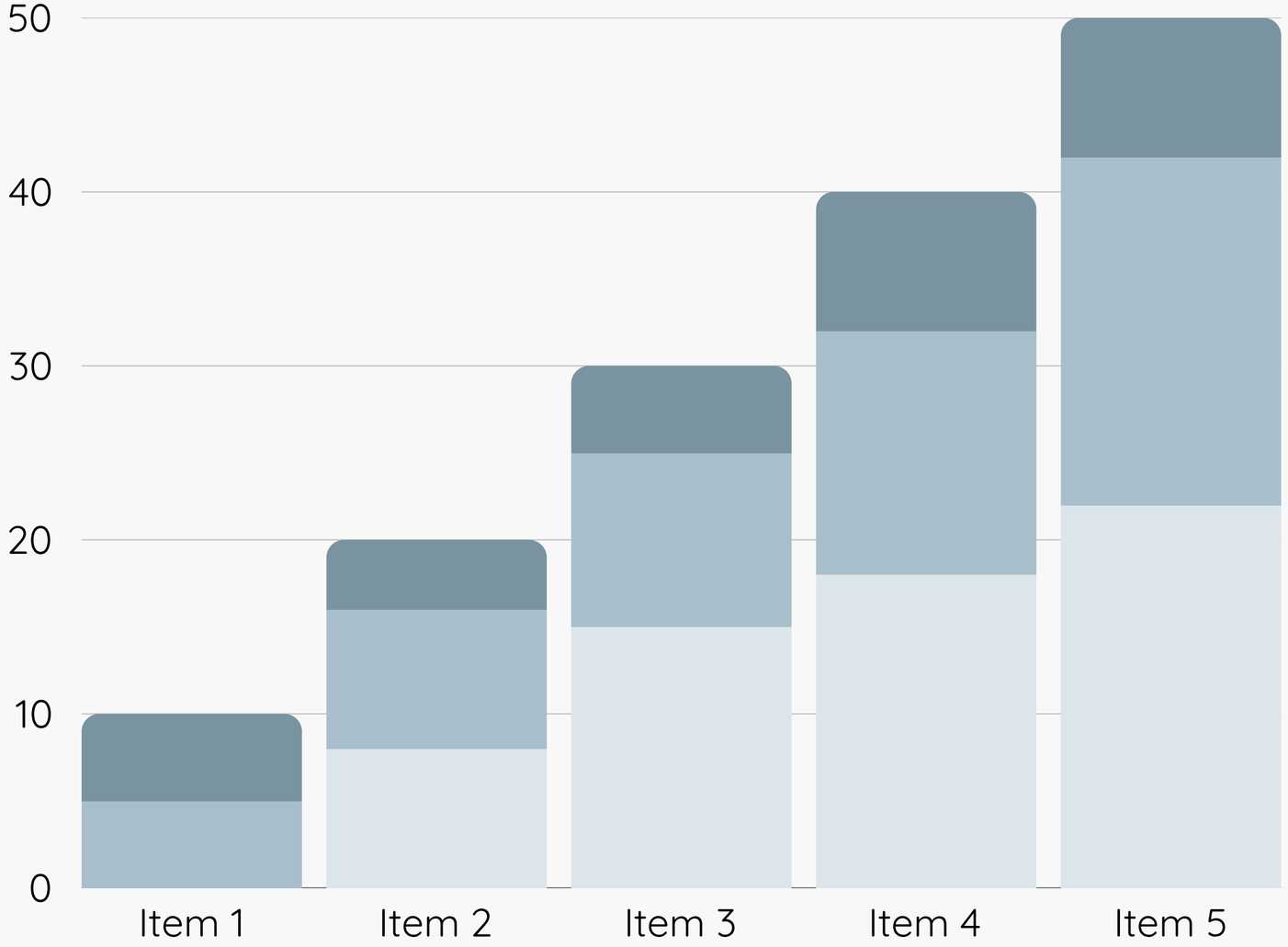


Next Months Plan...

- We aim to find more data and rather than the primary data generating it with the help of Thermocalc under controlled environments this will provide us a more range for study.
- We also prepare to work on the accuracy of the Data we generate

Thank you

Data Analysis



Over the past year, sales for Warner & Spencer have experienced a consistent decline, dropping month-on-month. The graphical representation of sales volumes reveals a noticeable downward trend, especially in the last quarter.

Product 1

Product 2

Product 3

Conclusion

By implementing a well-researched and innovative sales strategy, our goal is not only to boost immediate sales figures but also to establish a sustainable framework for continued growth and success.